ANSYS Fluent - Battery Discharge Simulation

ME 7260 – Project Report

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Table of Contents

List of Figures

List of Tables

Abstract

The primary focus of this simulation project was for our team to learn to use the ANSYS Fluent software, and to use that knowledge to replicate a tutorial given in class, as well as a research paper. This report will be structured in three parts. Part 1 will provide an overview of our successful replication of the provided tutorial. Part 2 will discuss the research paper that we replicated results from and explain some of the challenges that our group faced when running our simulation of the cylindrical battery. Finally, Part 3 will highlight how changing temperatures influences the discharge rate of a cylindrical battery cell, at a constant 4C.

This project required knowledge of battery cell systems, and the ability to use ANSYS Fluent to run battery simulations. Through this project, we simulated rectangular and cylindrical battery cells, and were able to run simulations on both types of batteries without crashes. Our data was consistent with our expectations based on discharge rates and temperature, so we feel confident that our simulations were run correctly.

Part 1- Replicating the Tutorial

In this first part of our project, our goal was to replicate the results of a simulation that was given to us as a tutorial, to better understand the ANSYS Fluent software. We were provided with a model and mesh, seen below in Figure 1.1.

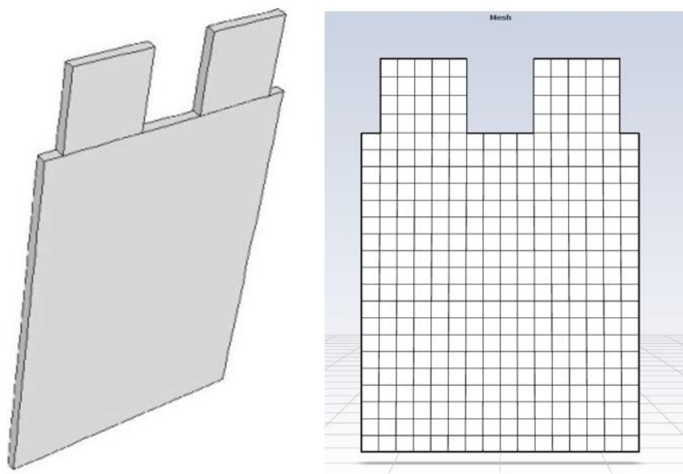


Figure 1.1 - Provided Model and Mesh

Using this model, we then set up our positive and negative tabs, as shown in Figure 1.2. This is an incredibly important step, as it dictates which tab will be the cathode, and which the anode.

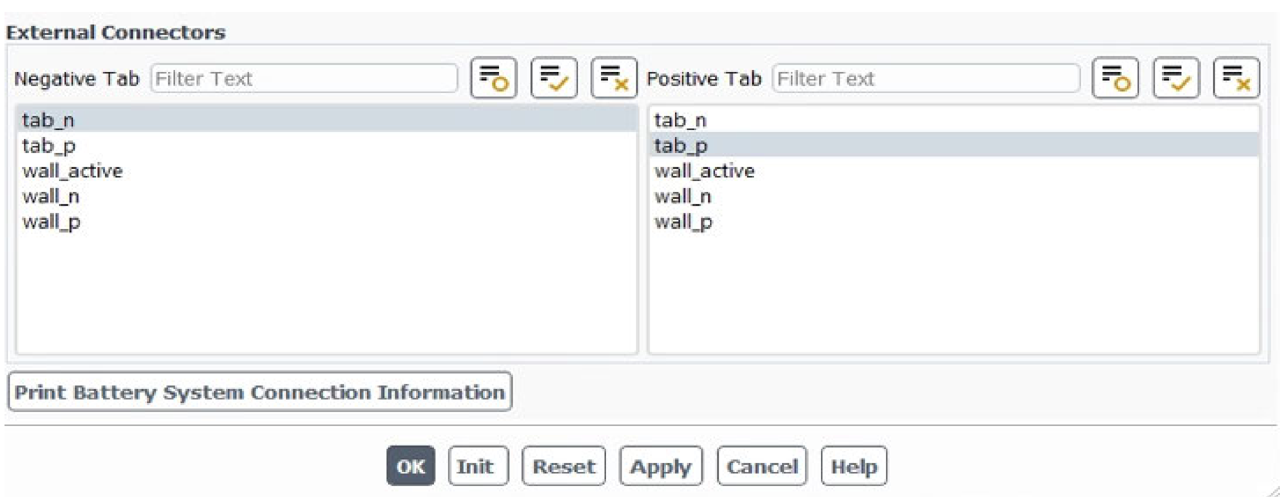


Figure 1.2 - Assigning electric contact to the connectors. Tab_n as negative and tab_p as positive

From this point, we assign materials to each wall, and designate the step size and number of steps for our simulation. The tutorial runs simulations at 1C, 0.5C, and 5C. A 1C simulation run for one hour. As such, 0.5C runs for two hours, and 5C should run for 12 minutes. Figure 1.3, below, shows the setup for our simulations at 1C, 0.5C, and 5C.

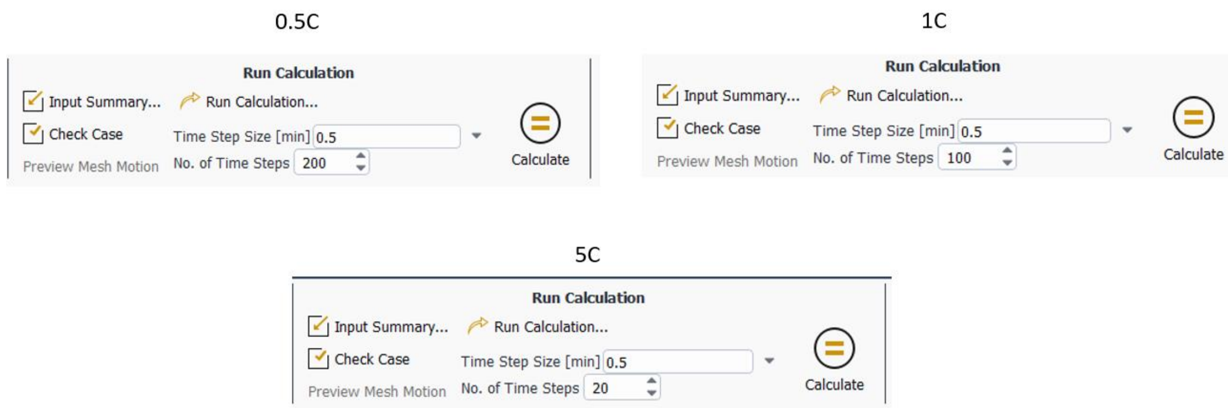
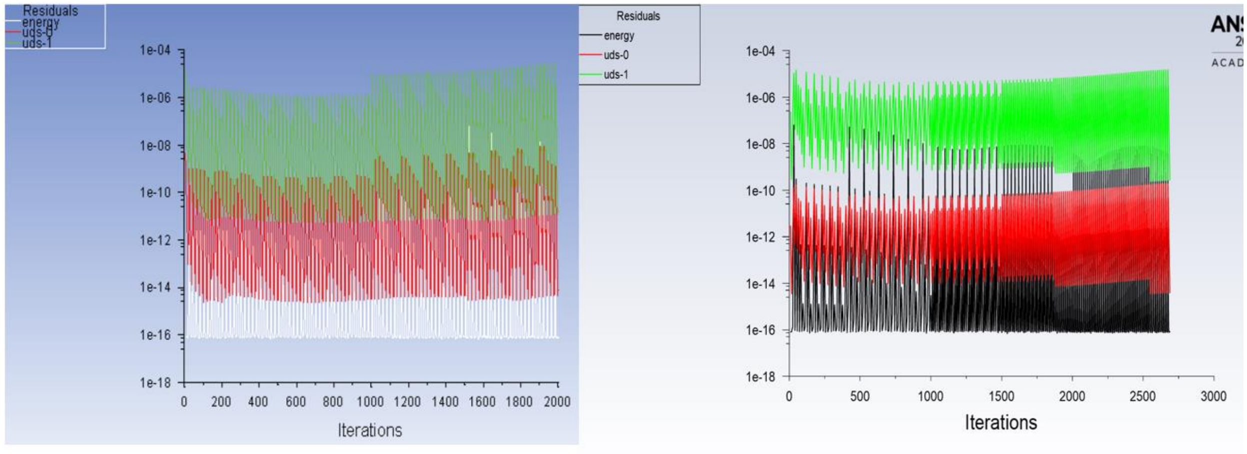


Figure 1.3 - Time steps to designate how long each simulation will run for

While it was stated that our simulations should be running for an hour for 1C, two hours for 0.5C, and 12 minutes for 5C, we were unable to run our simulations for those specified time lengths. For example, our step size was 0.5 mins, for 200 steps in 0.5C, or 100 mins. While 0.5C should be running for 2 hours, we ran into issues running for the full time. Our resultant graphs became unusable due to battery failure, as voltage and temperature went off the charts, skewing the results and changing the scale of our graphs. So, we ran our simulations for a little bit short of the full time, to show more detail in our results by ensuring that we did not run the battery until failure. For these same reasons, we ran our 1C for a total of 50 minutes, and our 5C for 10 minutes.

After initializing our model and running the calculation, we were able to accurately replicate the results that were given to us in the tutorial documentation. We created a residual history plot, contours for cathode and anode potentials, as well as temperature contour, graphs of temperature and voltage curves, as well as a vector plot of current densities. For the purposes of this paper, we will specifically be looking at a comparison of our results of simulations run for 1C against the results of the tutorial. Then, we will compare the temperature curves between our simulations at 0.5C, 1C, and 5C to discuss how the rate of discharge affects those parameters. All result plots and contours are available in Appendix A.

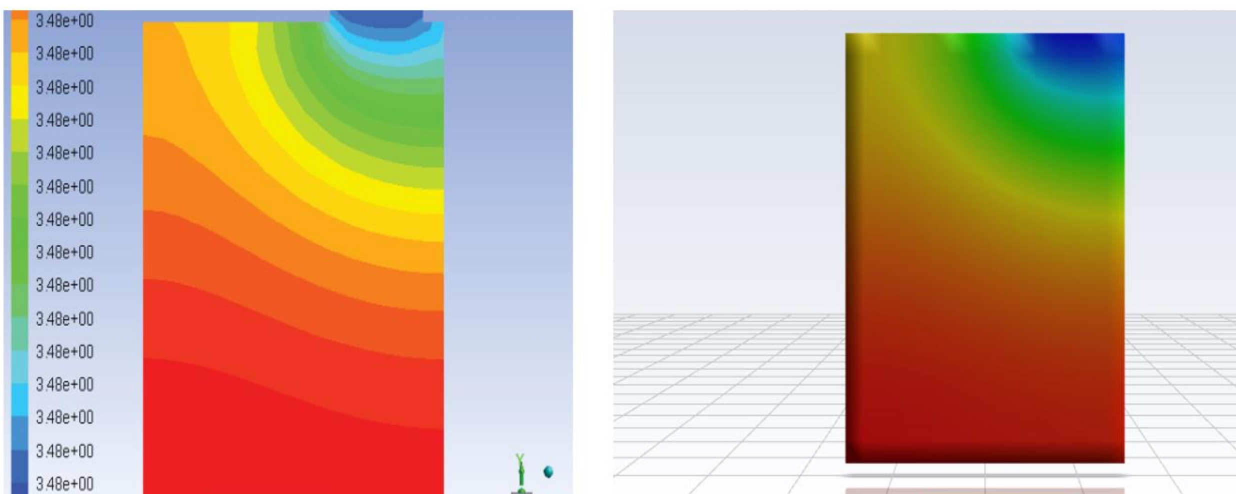
Comparison of Simulated and Tutorial Data for 1C



Tutorial   Simulation

Figure 1.4 - Comparison of Tutorial and Simulation Residual Histories

From Figure 1.4, we can see that both the tutorial and our simulation provided the same residual histories for energy, uds-0, and uds-1. We can see how our residuals increased in both plots as iterations were performed. With this plot, we can be sure that our simulation set up was done correctly, as the graph is replicated perfectly.



Tutorial   Simulation

Figure 1.5 - Comparison of Tutorial and Simulation Cathode Potential Contours

Figure 1.5 shows that the cathode potential trends in our simulation match those of the tutorial. We can be confident that we correctly designated our positive and negative tabs in our setup.

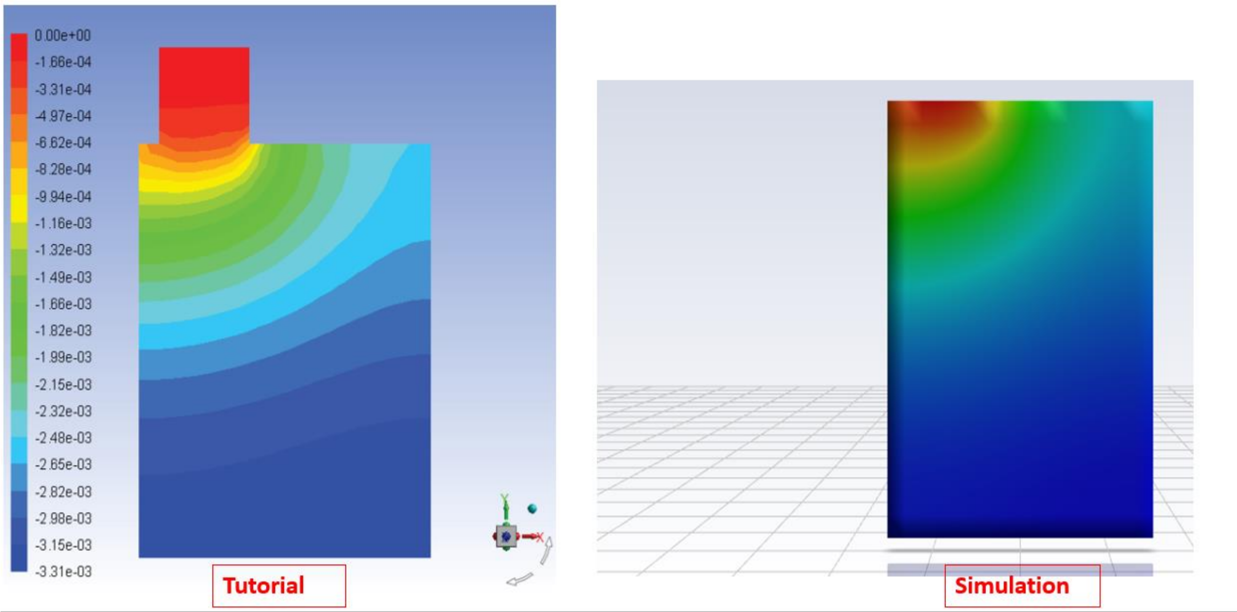


Figure 1.6 - Comparison of Tutorial and Simulation Anode Potential Contours

Figure 1.6 shows that the anode potential trends in our simulation match those of the tutorial. This reaffirms our understanding that we correctly designated our positive and negative tabs in our setup.

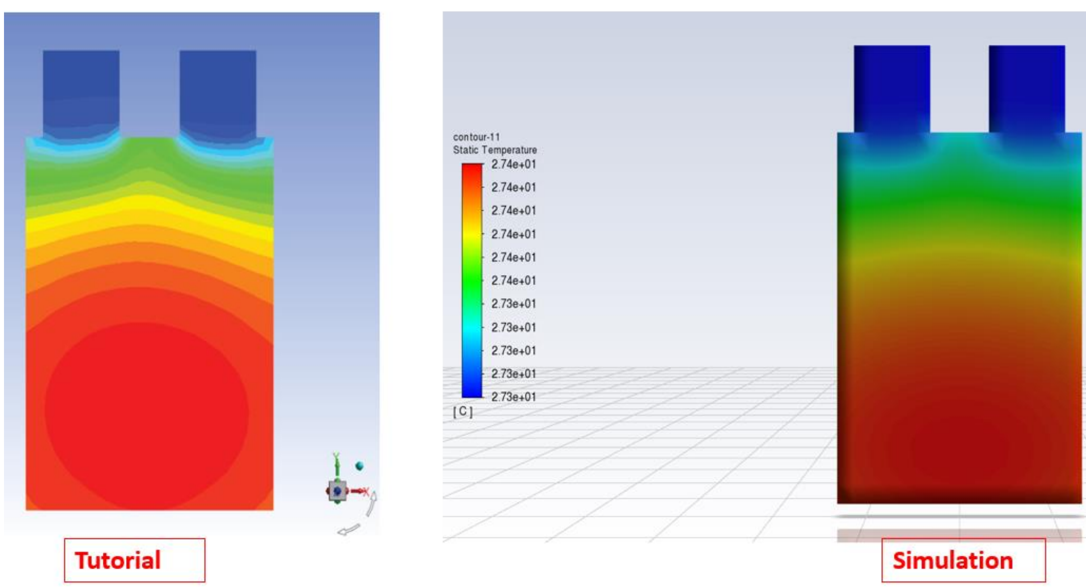


Figure 1.7 - Comparison of Tutorial and Simulation Temperature Contours

Figure 1.7 shows that our temperature contours matched with the tutorial results. We can safely assume that all our boundary setups were done properly, based on this replication.

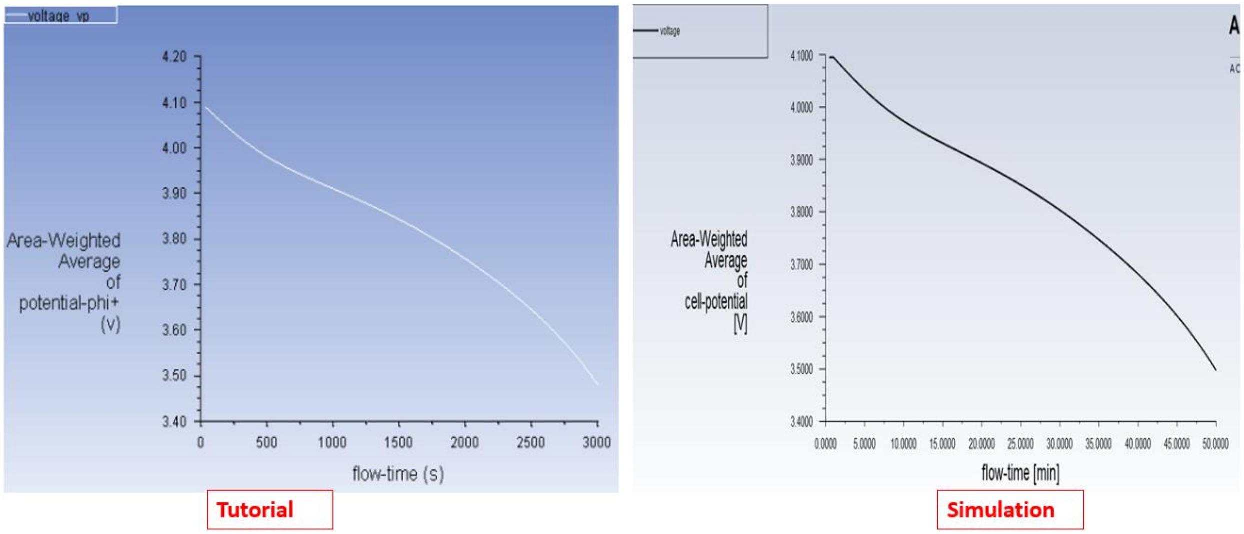


Figure 1.8 - Comparison of Tutorial and Simulation Voltage Curves

Figure 1.8 is a good indication that the simulation was run properly. We can see an exact replication of the tutorial voltage curve. Starting and ending values are consistent, the profile of the curve is the same.

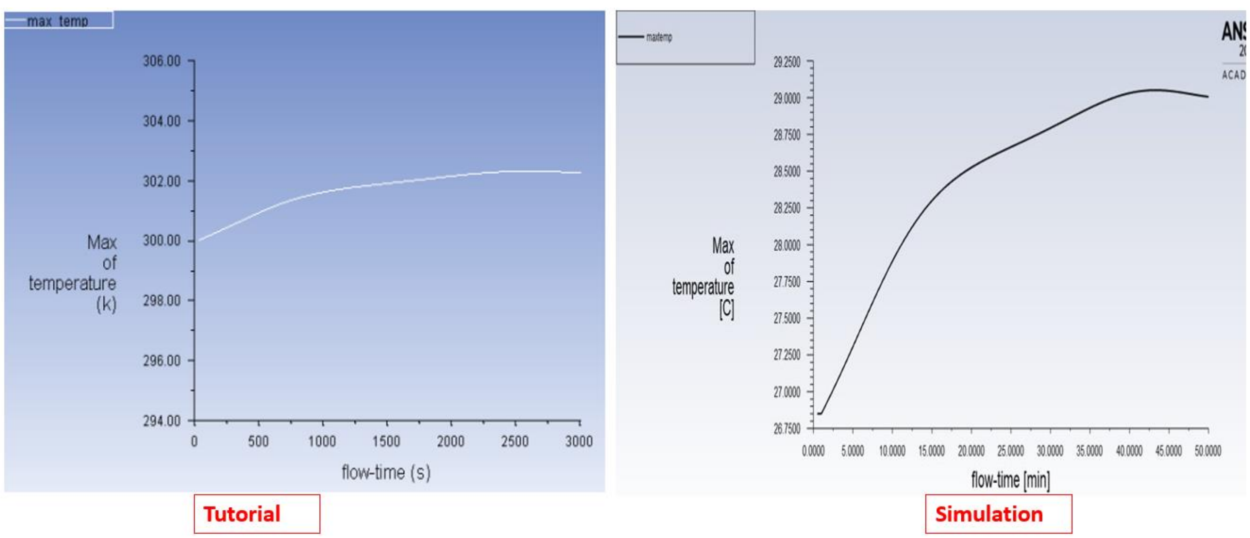
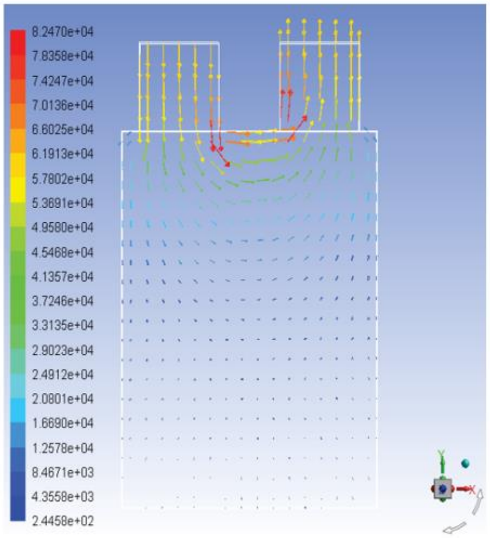
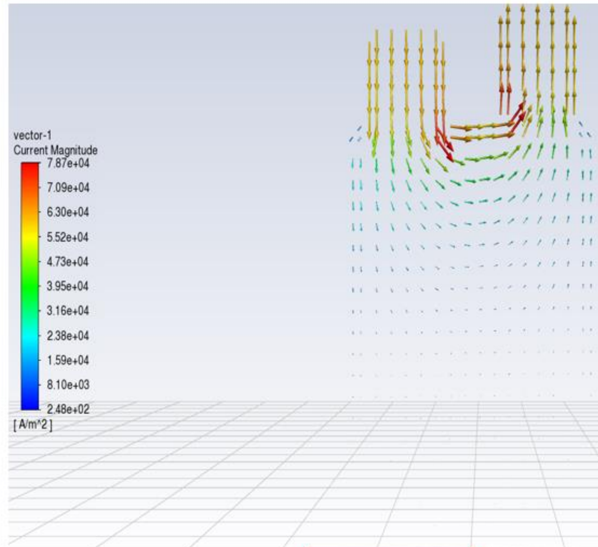


Figure 1.9 - Comparison of Tutorial and Simulation Max Temperature Curves

While the two plots in Figure 1.9 do not look the same, this is because of unit discrepancies. The tutorial used Kelvin units, while our simulation used Celsius. After a conversion, the numbers match up perfectly. Additionally, the profiles of the plots look different, but this is due to scale differences in the graphs. The numbers match up exactly, and by looking at the results from Figures 8 and 9 together, we can feel confident that we were able to accurately replicate the simulation.



Tutorial



Simulation

Figure 1.10 - Comparison of Tutorial and Simulation Current Density Vector Plots

Current density showed correct direction of the vectors, so we can feel secure that we correctly set up anode and cathode. While the numbers do not match up exactly, they are very close, and we can explain this difference due to software version and missing options in the setup menu. Overall, this current density vector comparison shows us that everything was set up correctly, and the battery behaves as expected.

We have shown that our team was able to correctly replicate the tutorial simulations. Our contours, graphs, and vector plots are all consistent with the tutorial results. While our paper has focused on the comparison of 1C data, all resultant plots of our 0.5C and 5C data are available in Appendix A. We will now compare the temperature plots from the three simulations to understand how the discharge rate affects the maximum temperature of the battery under operation.

Comparison of 1C, 0.5C, and 5C Maximum Temperatures

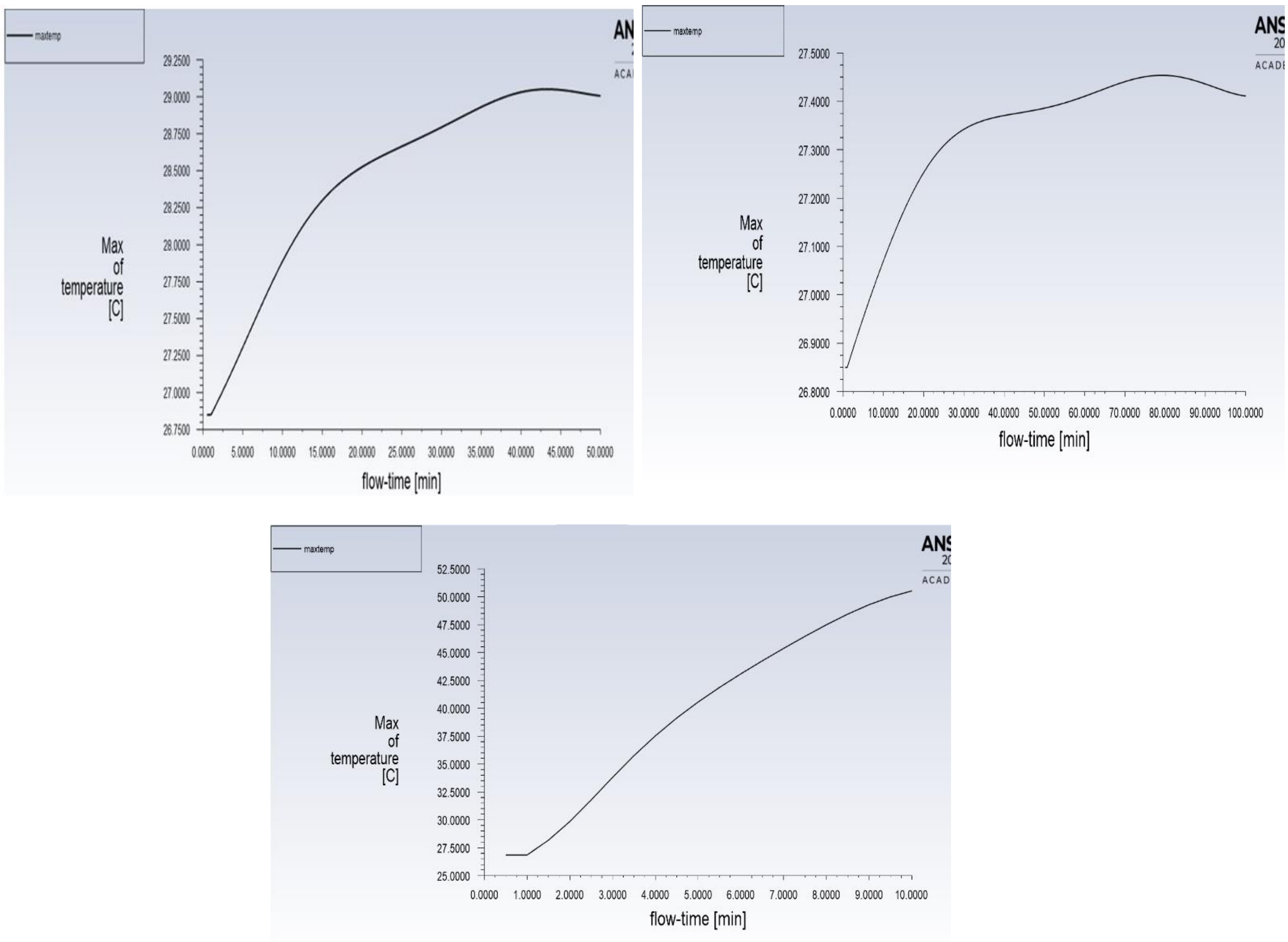


Figure 1.11 - Comparison of Temp. Plots from 1C (upper left), 0.5C (upper right) and 5C (bottom)

Notable differences between these plots are the slopes and temperature values. We can see that 1C and 0.5C held a similar profile, and that the 1C plot had maximum temperature of a degree higher than 0.5C. The largest differences come when we compare 0.5C to 5C discharge rates. We see temperatures at 5C skyrocket to over 50°C, compared to 27 °C in 0.5C case. This shows that the discharge rate (ten times higher in this case) plays a large part in creating heat within the battery cell. This is consistent with common logic; if the battery cell is being discharged (energy being used) at a faster rate, the battery will get hotter and more quickly than if being used until discharge over a longer period.

Part 2- Replicating Research Paper and Creating a Cylindrical Battery Cell

Comparison of Rectangular and Cylindrical Battery Cells

Before moving into a discussion about our research paper and replication using a cylindrical battery, it is important to note the differences between the rectangular battery that we used in Part 1 and cylindrical batteries, which will be the focus of the remainder of this report. A clear difference is the shape and structure of the batteries themselves. The rectangular battery is simple, and as it is flat, it is extremely versatile is making custom sizes to fit any need. For this reason, many electric vehicles feature rectangular batteries for their power source. As you can see from Figure 2.1, the design of this type of battery is relatively simple, with the positive and negative terminals on top, and a shell surrounding the electrolyte material. These batteries tend to have very high energy density and are extremely light, as there are fewer accessories when compared to its cylindrical counterparts. However, the convenience and versatility of rectangular batteries has made it difficult to unify, as there are thousands of custom sizes available. For large scale industrial equipment that require many batteries in series or in parallel, ensuring that all batteries are standardized is incredibly important, and cylindrical batteries may be a better option.

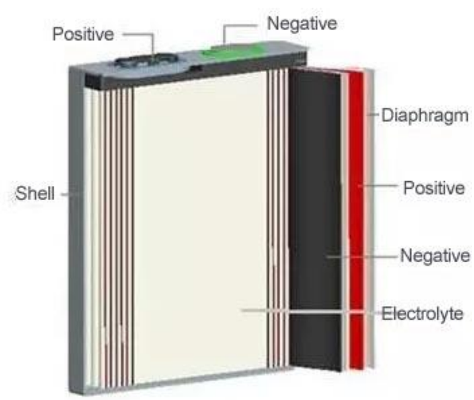


Figure 2.1 - Overview of the structure of a typical rectangular lithium-ion battery (Grepow, 2019)

In contrast, cylindrical battery cells are far more complex. The negative and positive terminals are located at the bottom and top of the cell respectively. Because of the standardized shape, it is easy to mass manufacture, and is ideal for scenarios that require linking multiple batteries in series or parallel. However, these batteries have lower energy density than their rectangular counterparts, and as such, are less efficient for use in electric vehicles. As noted in Figure 2.2, cylindrical batteries have been outfitted with numerous safety accessories such as vents and explosion-proof safety valves. These accessories add weight to the battery, another reason while they are less ideal for vehicles.

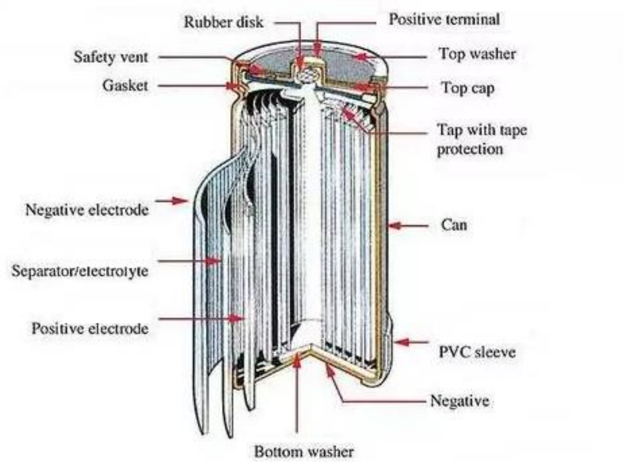


Figure 2.2 - Overview of the structure of a typical cylindrical lithium-ion battery (Grepow, 2019)

Our limited knowledge of ANSYS Fluent made modelling all these safety components incredibly difficult. Our team ran simulations by replicating the process of creating a rectangular battery and applying that concept to our cylindrical battery. As such, these safety features are not included in our simulation, which can explain some discrepancies between the experimental and simulation data, as we will discuss later in this Part 2.

To fully understand Fluent and the MSMD battery model, we researched a couple of papers that had data for discharge with battery dimensions. We ended up picking a paper by Edoardo Catenaro and Simona Onori from the Department of Energy Resource Engineering, Standford University. This paper contained "Experimental data of lithium-ion batteries under a galvanostatic discharge test at different rates and temperature of operation." Six samples of three different batteries were tested. Each had the same anode composition, but the cathode composition varied between them. For simplicity and to complete our objective of comparing the simulation with the results, the Panasonic NCR-18650B was selected. Its cathode composition was made from lithium-nickel-cobalt aluminum-oxide (NCA). See next page.

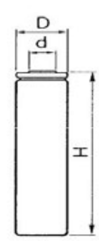
Nominal voltage (V)	3.6
Nominal capacity*1 - Minimum (mAh)	3,250
Nominal capacity*1 - Typical (mAh)	3,350
Dimensions - Diameter (mm)	18.5
Dimensions - Height (mm)	65.3
Approx. w^eight (g)	47.5

Figure 2.3 - Panasonic NCR-1860B NCA Battery and its Parameters

Battery Model, Mesh, Parameters, Materials and Run Calculations

To replicate this as a model, three bodies were created in Autodesk Fusion 360 and exported as .step files into DesignModeler by ANSYS. There was a separate body for the positive tab, negative tab, and the battery itself which matched the dimensions provided (see below and next page). From there, a mesh with roughly 3600 nodes was created and imported into Fluent for the battery calculation. Battery model parameters such as capacity, temperature, C rate, timesteps were modified accordingly for each iteration.

Cell Type NCR18650B



Dimensions(Typ.) of Bare Cell		
	H	64.93mm
	D	18.2mm
	d	7.9mm

Discharged State after Assembling

Specifications

Rated Capacity (at 20℃)		Min.3200mAh
Nominal Capacity (at 25℃)		Min.3250mAh
		Typ.3350mAh
Nominal Voltage		3.6V
Charging Method		Constant Current -Constant Voltage
Charging Voltage		4.2V
Charging Current		Std.1625mA
Charging Time		4.0hrs.
Ambient Temperature	Charge	+10～+45℃
	Discharge	-20～+60℃
	Storage	-20～+50℃
Weight (Max.)		47.5g
Dimensions (Max.) Maximum size without tube	(D)	18.25mm
	(H)	65.10mm
Volumetric Energy Density		676Wh/l
Gravimetric Energy Density		243Wh/kg

2G23X0KYKU

Panasonic ideas for life

Figure 2.4 - Specifications of Panasonic NCR-18650B NCA Battery

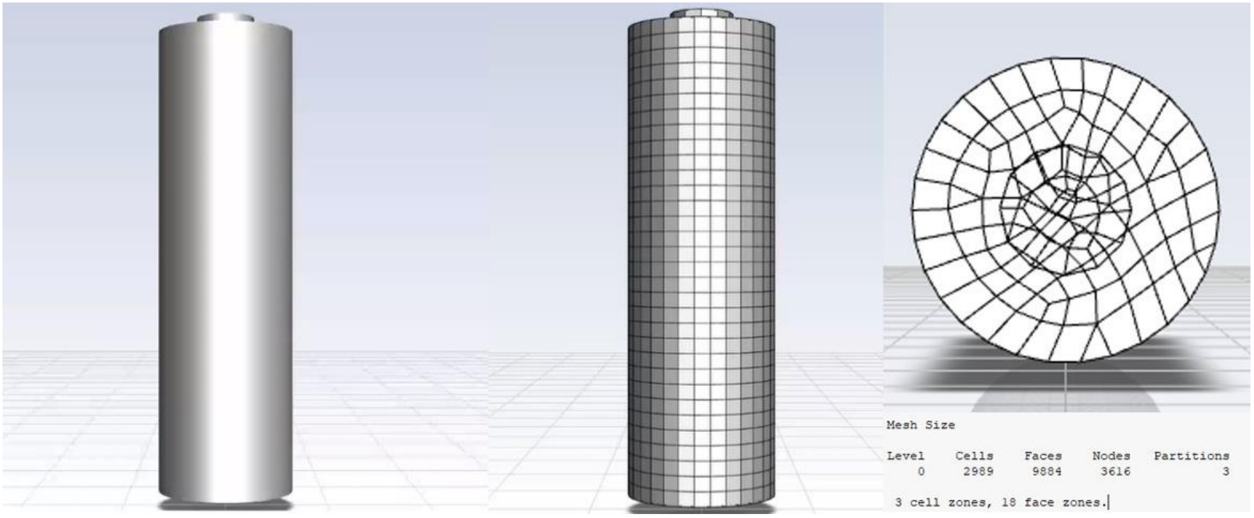


Figure 2.5 - Cylindrical Battery Mesh

The above figure illustrates the battery mesh which only contains solid elements. In Figure 2.3, we see that there are 11 components in a physical cell, and this was not quite possible to model with our setup. This is also why some of our results did not accurately match with the data provided and will be discussed later. A key fundamental to how Panasonic Li-Ion batteries work is that they deploy a Heat Resistance Layer (HRL) which improves the batteries safety and prevents it from overheating (see below)

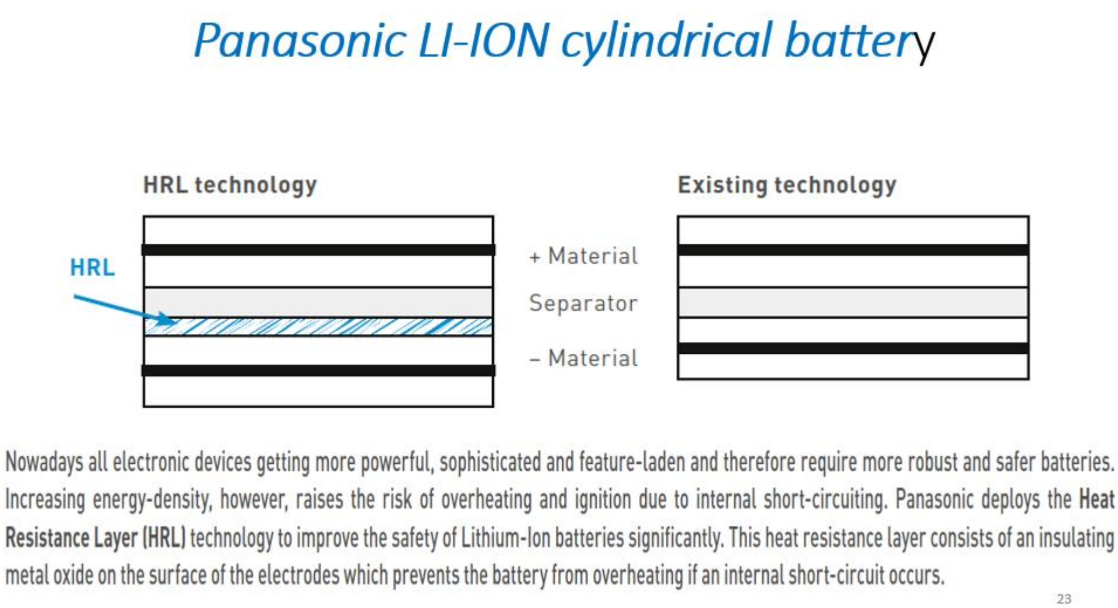


Figure 2.6 - Panasonic Li-Ion Heat Resistance Layer

Only the Nominal Cell Capacity [ah] was modified to 3.35 to match that of the NCA battery as shown below. Every other parameter was unchanged except for the C rate for each iteration in this configuration window.

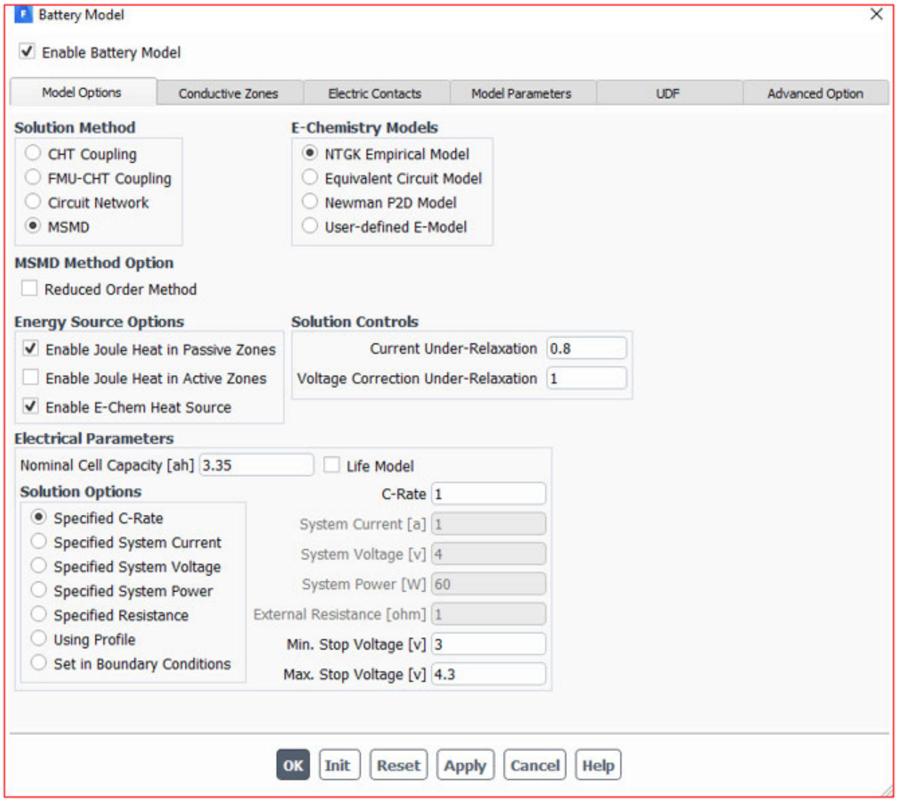


Figure 2.7 - Battery Model Parameters

Our paper suggested to use graphite-based anode and lithium-nickel-cobalt aluminum oxide for cathode and after doing some trial runs, we determined that the bodies for positive tab and negative tab were too small to make an impact to the results. We kept these as the same as the tutorial. Note e_material was applied to the body and both tabs (copper) were applied to the n_material/p_material (tabs).

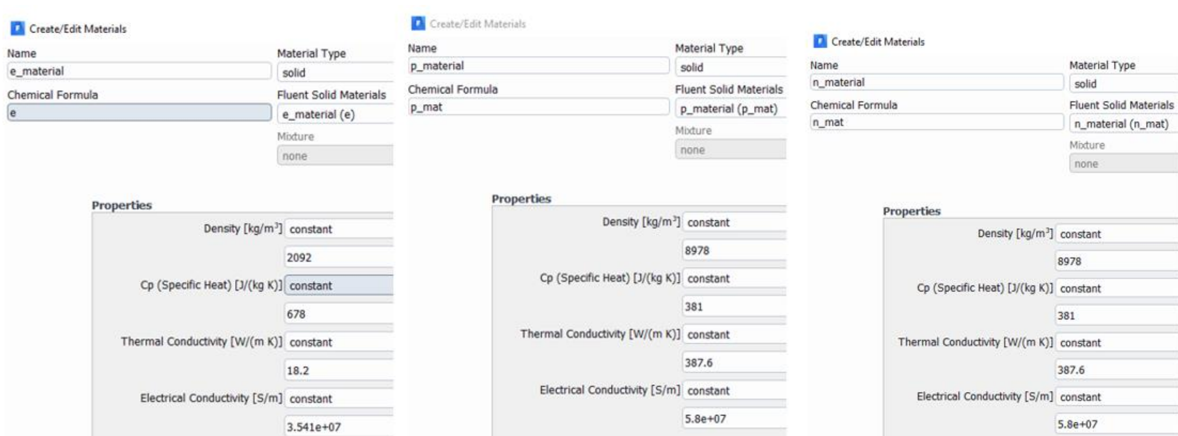


Figure 2.8 - Battery Materials

The following table illustrates the number of timesteps each C rate was run at.

Battery Run Calculations		
C Rate	Time Step Size [min]	Number of Time Steps
1C	0.5	110
2C	0.5	55
3C	0.5	36
5C	0.5	22

Table 2.1- Cylindrical Battery Model Run Calculations

Cylindrical Battery Simulation Results at 25°C

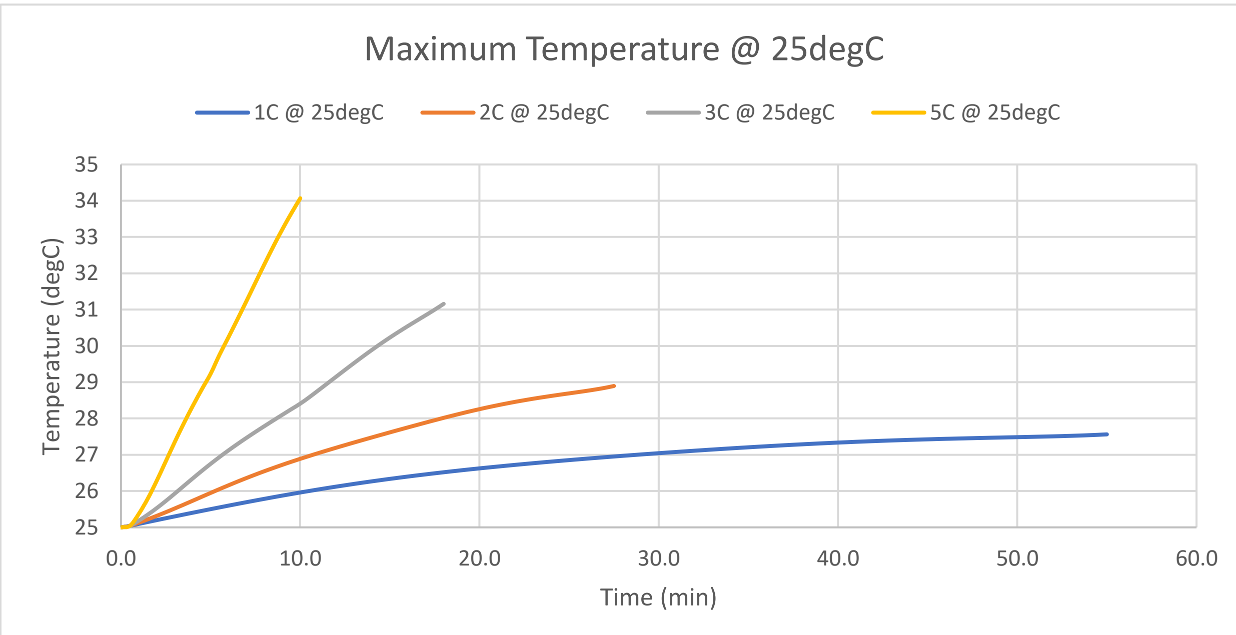


Figure 2.9 - Temperature Curve of 1C, 2C, 3C, 5C at 25°C

When looking at the results for the temperature, we note several things. We notice that 1C peaks at roughly 27.5°C at 55 mins and 5C peaks at 34°C at 10 mins with a starting temperature of 25°C for both. From this we can conclude that the increase in C rate is directly proportional to the temperature rise and inversely proportional to the time. The time decreases as C rate increases. Also, it should be noted that the temperature curve gets more linear as the C rate increases.

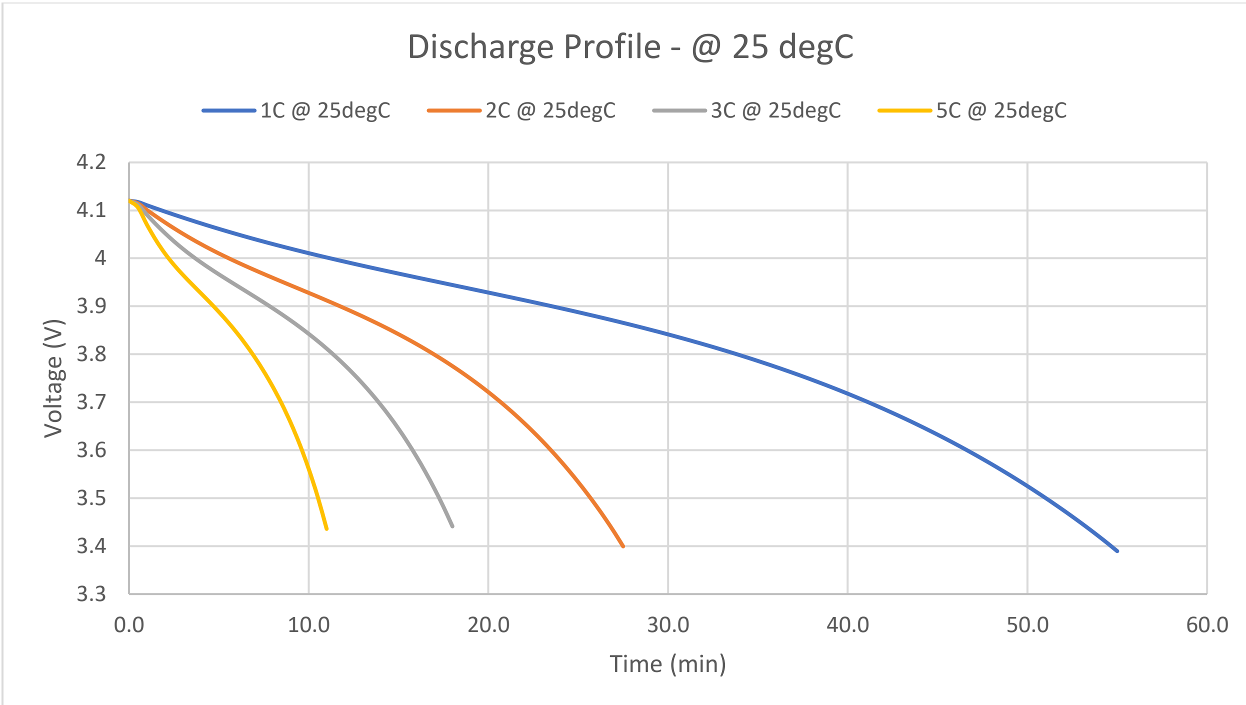


Figure 2.10 - Discharge Profile of 1C, 2C, 3C, 5C at 25°C

The voltage graph above indicates a similar curve pattern for each C rate. We notice that each curve starts at a voltage of 4.1V and drops to 3.45-3.39V. Unlike Figure 2.9, both voltage and time are inversely proportional to the C rate.

Below are contour images for cathode and anode potential, and static temperature. The contours for cathode and anode potentials do not depict a major change between 1C-5C. For cathode potential, the ranges are similar. Anode potential on the other hand varies but in very small increments of 10^-5.

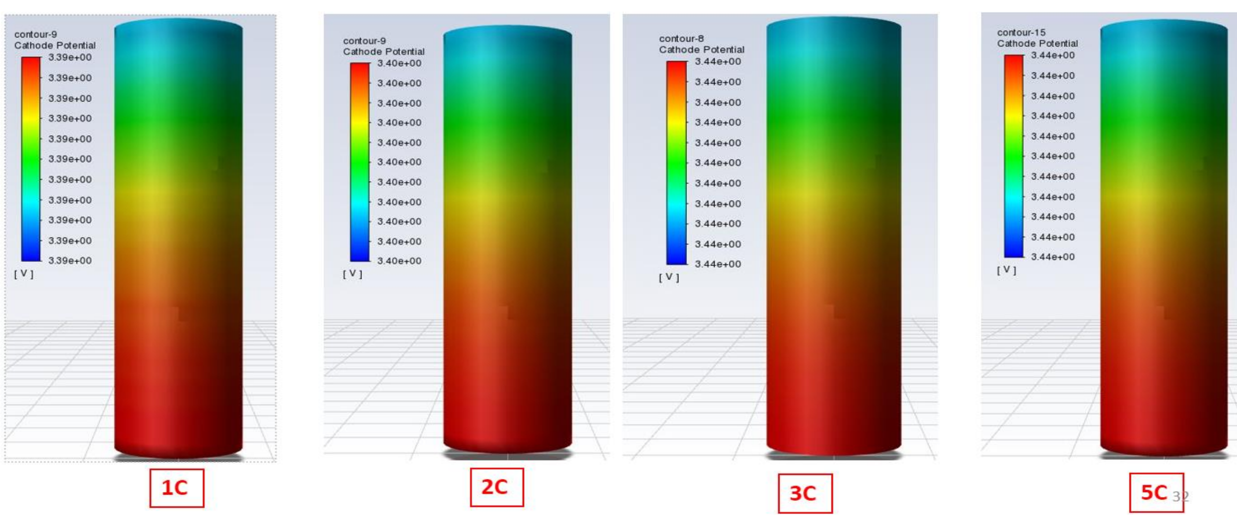


Figure 2.11 - Cathode Potential for 1C, 2C, 3C and 5C

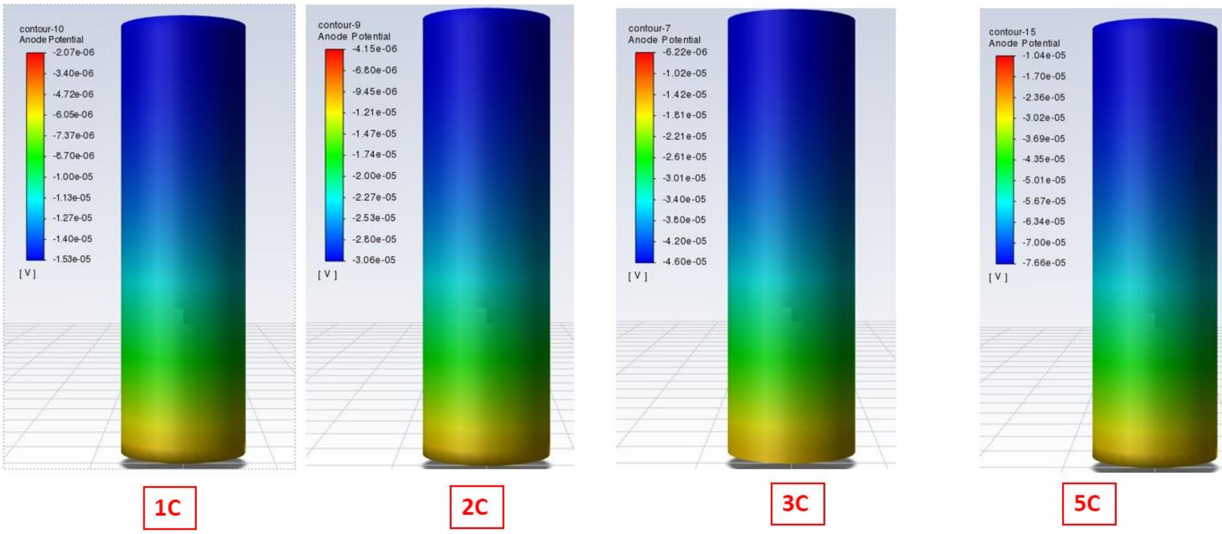


Figure 2.12 - Anode Potential for 1C, 2C, 3C and 5C

Static temperature is an area where we notice some significant differences. As expected, the contours behave like the temperature curves as indicated in Figure 2.9 and increase directly proportional to C rate. Although the scale is static, we notice a significant contour difference with 5C as compared to the other C rates. The cathode portion, or the top portion of the cylindrical battery, shades from a blueish color whereas the others start at a greener color. This may be an indication that although we cannot see a numerical scale difference, there is variation and that perhaps the increments are too small, and the scale is formatted to a certain significant digit. This static temperature contour does not indicate which timestep it corresponds to.

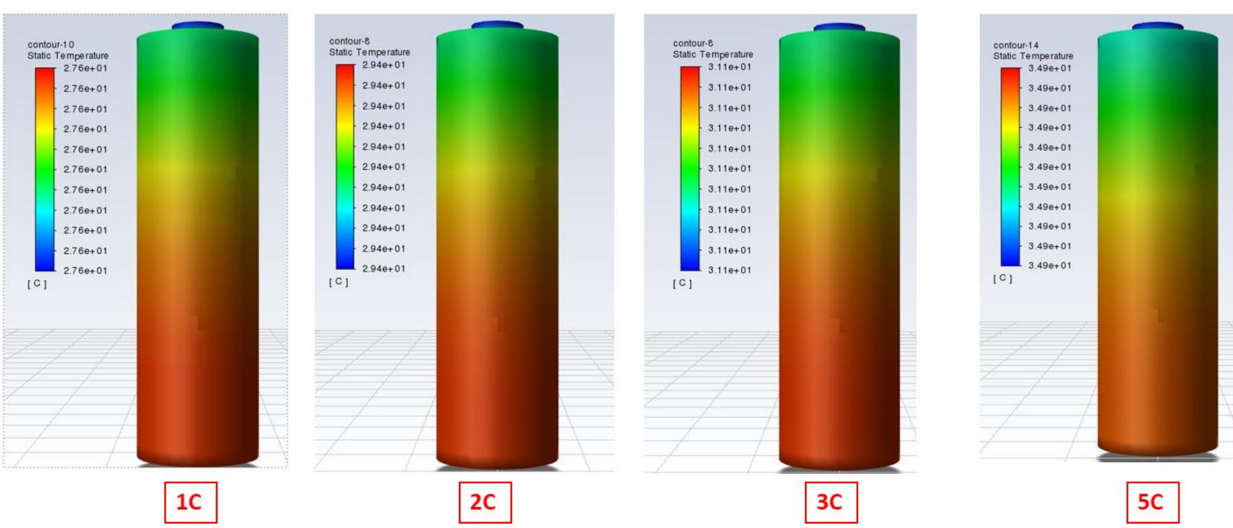


Figure 2.13 - Static Temperature of 1C, 2C, 3C and 5C

Discharge Profile and Maximum Temp. Comparison; Data vs. Simulation

Data for discharge profiles was provided for several C rates (denoted as "Voltage(V)_exp") and are plotted against the simulation data (denoted as "Voltage(V)_mod"). We tried to mimic the duration of each C rate by inputting as many timesteps as we could without having our simulation crash.

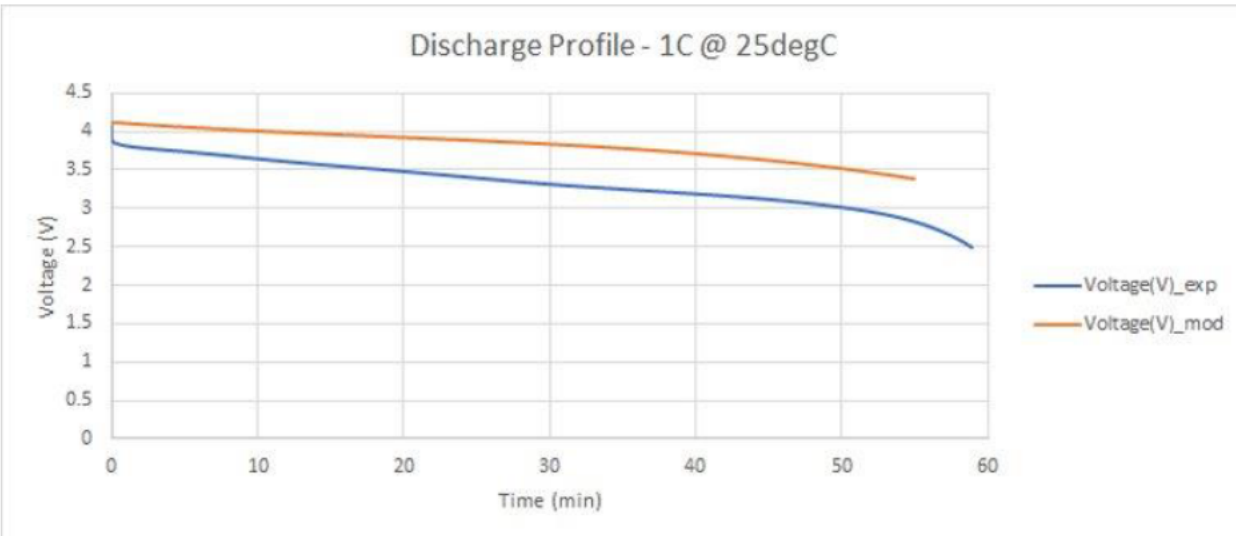


Figure 2.14 - Discharge Profile of 1C at 25°C

The figures above and below illustrate the discharge profile for 1C at 25°C and maximum temperature from our simulation and data provided. Our results seem very similar and generally follow the trends of the data provided, with slight offsets. The data provided ran for 5 more minutes and we were not able to do this because our simulation would crash. If this were not the case, we are certain that voltage for 1C would decrease in a similar manner and temperature would spike towards the end.

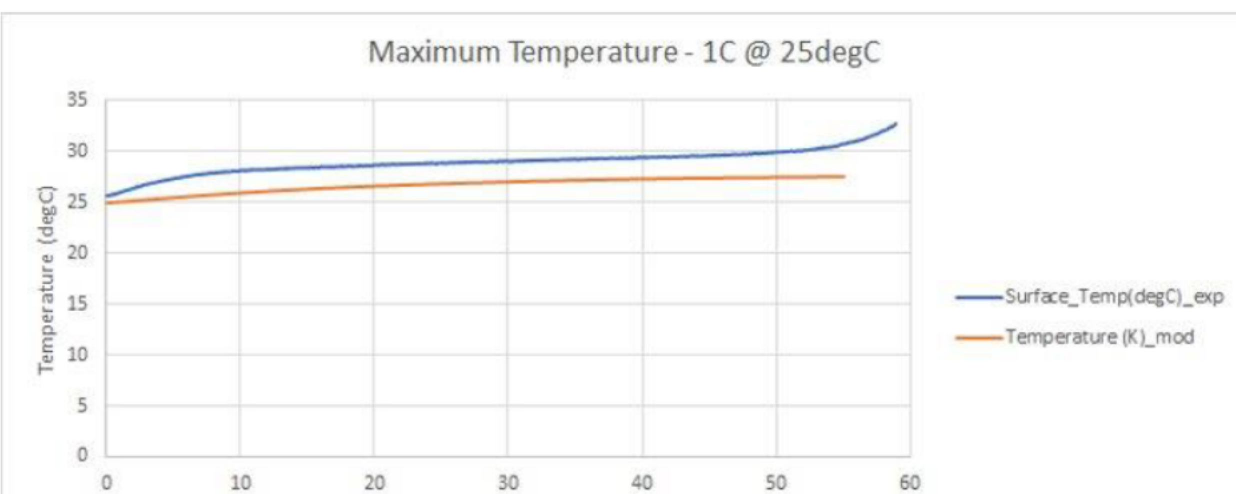


Figure 2.15 - Maximum Temperature of 1C at 25°C

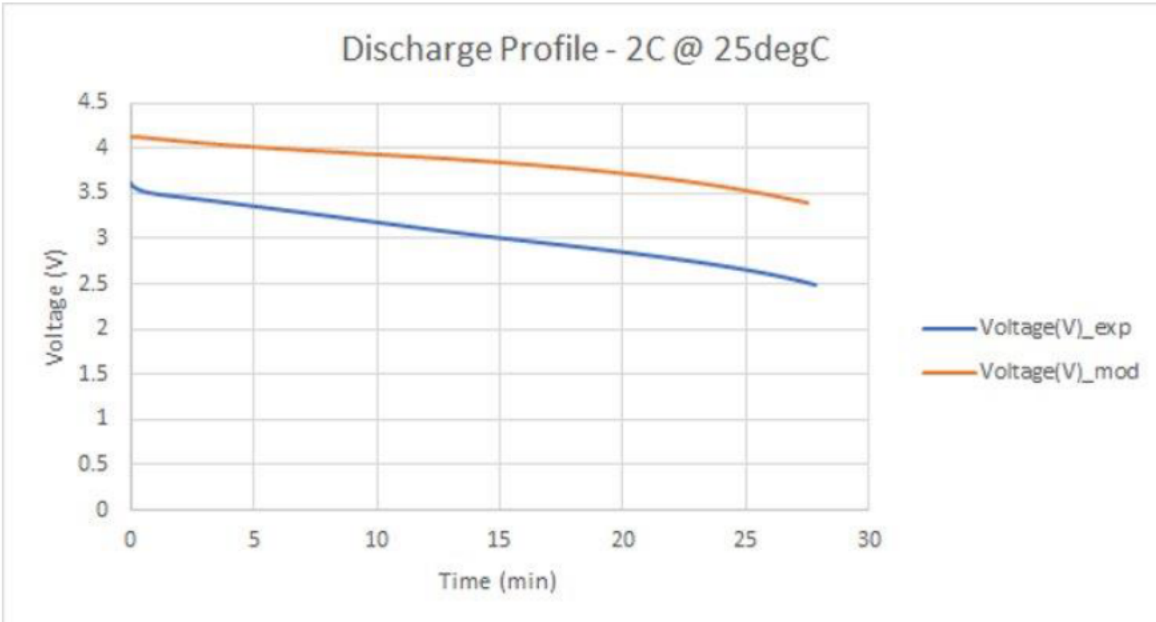


Figure 2.16 - Discharge Profile of 2C at 25°C

The figures above and below illustrate the discharge profile for 2C at 25°C and maximum temperature. For discharge, we can observe an offset of .5V between the two curves and we believe this may be due to the battery model not being 100% representative of the physical battery. Again, our mesh is only a solid and a physical NCA battery contains multiple components. If we neglect this, our curve slope, trend, and patterns can be perceived to be the same. For maximum temperature, our simulation curve follows a linear trend whereas the data provided curve is polynomial and peaks out at a higher temperature. The difference in trends is related to the battery model setup.

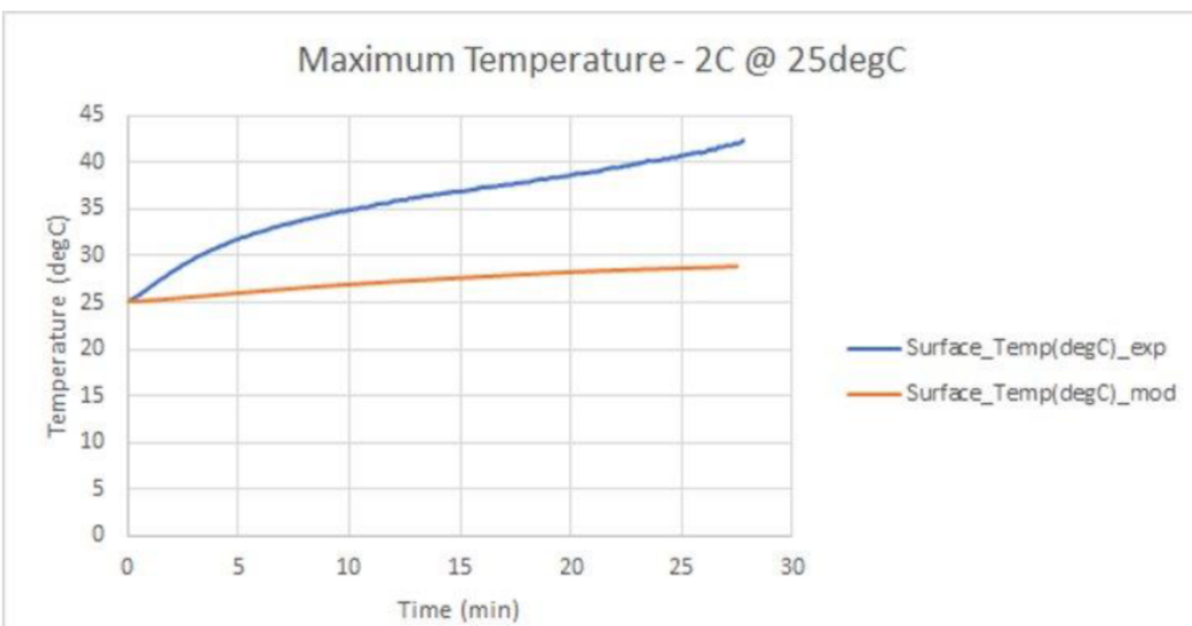


Figure 2.17 - Maximum Temperature of 2C at 25°C

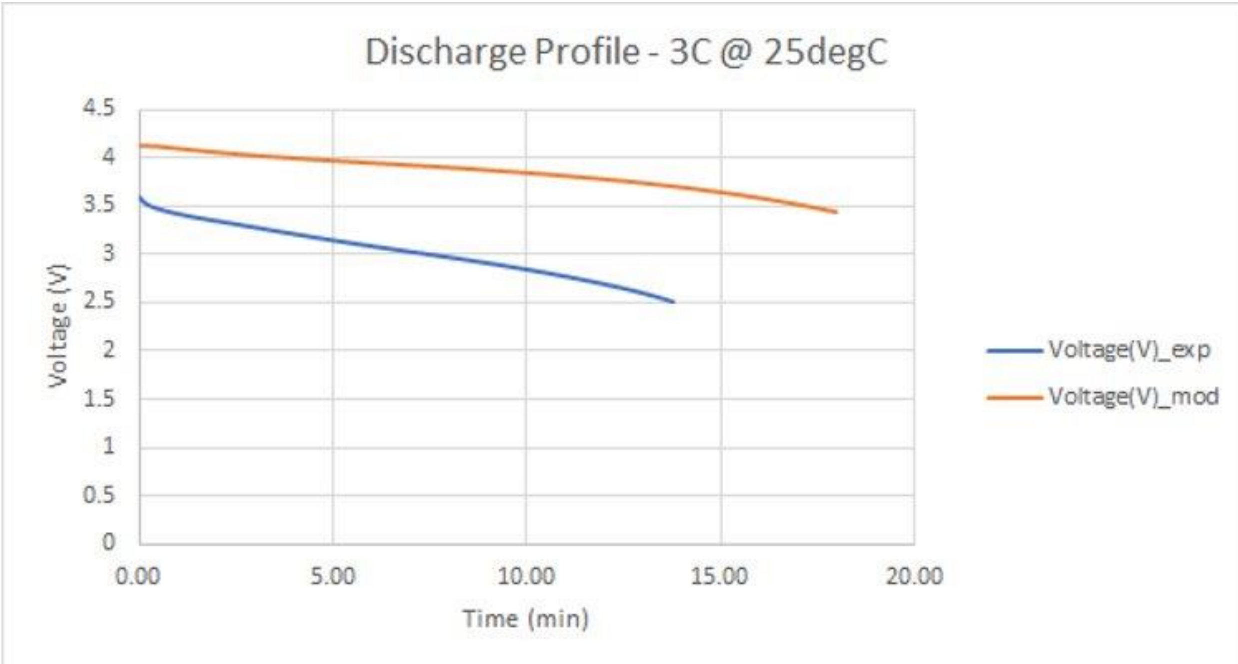


Figure 2.18 - Discharge Profile of 3C at 25°C

The figures above and below illustrate the discharge profile for 3C at 25°C and maximum temperature. For discharge, we can observe an offset ranging from .5V and eventually increasing to 1V at 11 mins between the two curves. Again, our mesh is only a solid and a physical NCA battery contains multiple components. If we neglect this, our curve slope, trend, and patterns can be perceived to be the similar. For maximum temperature, our simulation curve follows a linear trend whereas the data provided curve is polynomial and peaks out at a higher temperature. The differences in trends is related to the battery model setup.

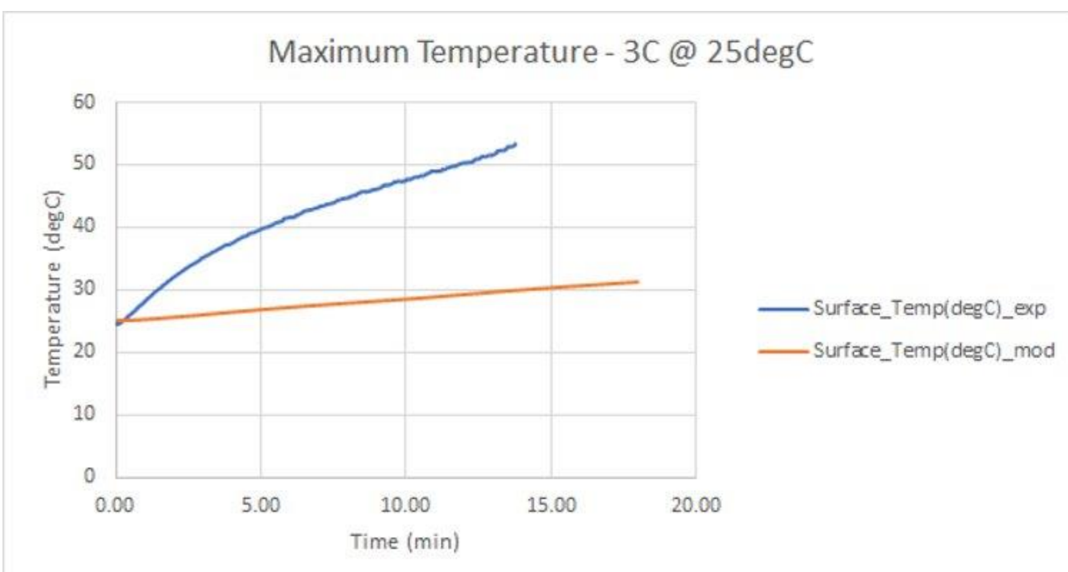


Figure 2.19 - Maximum Temperature of 3C at 25°C

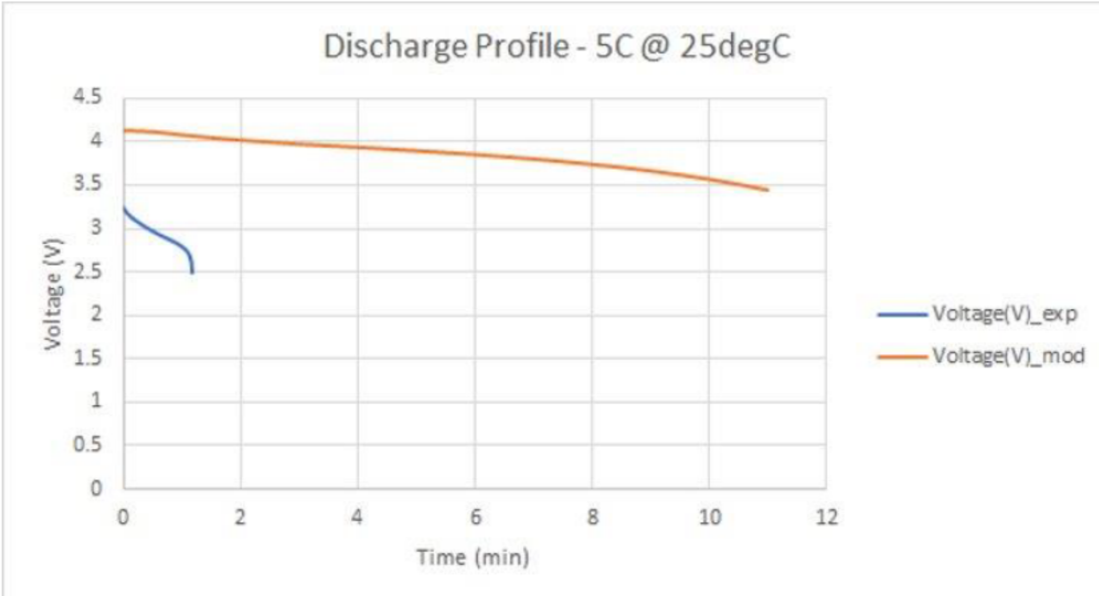


Figure 2.20 - Discharge Profile of 5C at 25°C

The figures above and below illustrate the discharge profile for 5C at 25°C and maximum temperature. For discharge, it is obvious that the two curves are not very similar, follow different trends and end at different times. Our simulation runs for 11 mins whereas the data provided is only 1 min. Again, our mesh is only a solid and a physical NCA battery contains multiple components. For maximum temperature, both simulation and data provided curves start and peak at around ~35°C. These curves also differ by 10 mins and the differences here can be linked with the battery model setup.

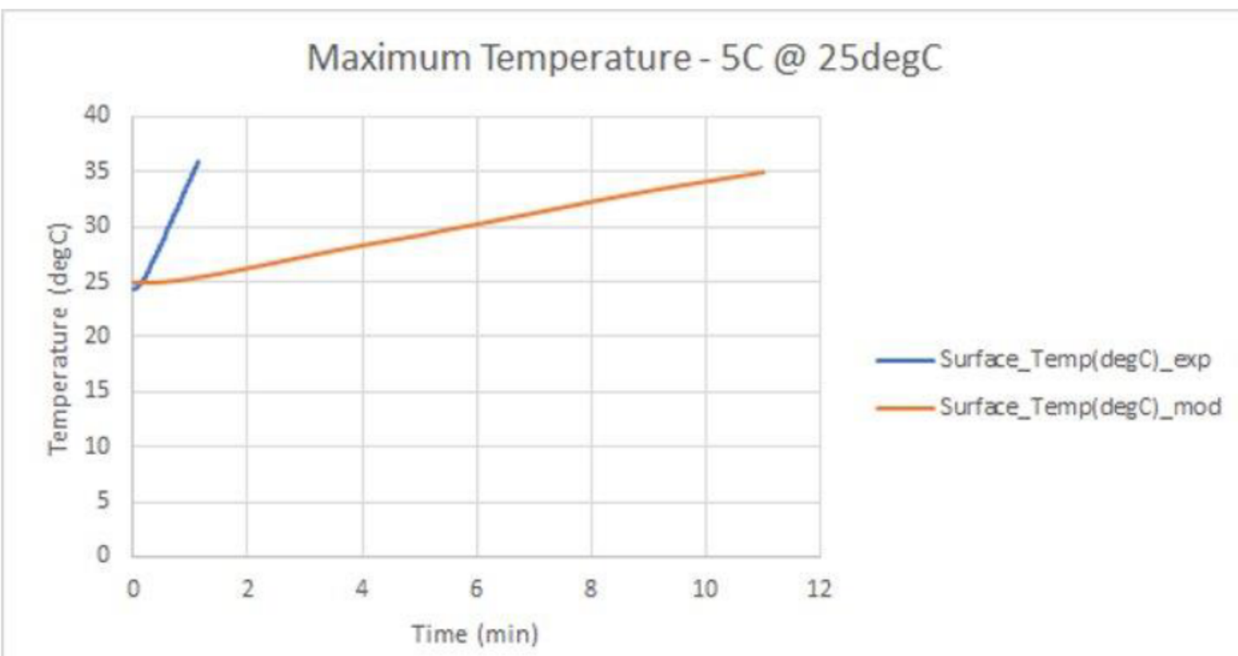


Figure 2.21 - Maximum Temperature of 5C at 25°C

Curve Fitting

The experimental data provided contained six samples of data. In the paper, these are referred to k1, k2, k3, etc. We obtain data only for k1 at step index 5 and compare it with our simulation. Step index 5 is when Galvonostatic Discharge occurs (discharge current applied according to the C-rate) – refer to Table 2.1 of paper. The reason we did not average all the k1-k6 samples for step index 5 was because the number of time steps were inconsistent. See below:

	A	B
1	Step_Time(s)	Voltage(V)
1661	1660.0002	2.510688782
1662	1661.0002	2.509513617
1663	1662.0002	2.508351326
1664	1663.0012	2.5070467
1665	1664.001	2.505755186
1666	1665.0004	2.50438118
1667	1666.0012	2.503071308
1668	1667.0006	2.501931667
1669	1668.0007	2.500630617
1670	1668.4063	2.499984741

K1 step index 5 has 1670 steps

	A	B
1	Step_Time(s)	Voltage(V)
1812	1811.0012	2.555276632
1813	1812.0008	2.550895929
1814	1813.0013	2.546502352
1815	1814.0011	2.541854858
1816	1815.0009	2.537136555
1817	1816.0009	2.532325029
1818	1817.0003	2.527327776
1819	1818.0003	2.52218008
1820	1819.0013	2.517088175
1821	1820.0007	2.511617422
1822	1821.0009	2.506258011
1823	1822.0011	2.500784636
1824	1822.1147	2.499963045

K5 step index 5 has 1824 steps

Figure 2.22 - K1 vs K5 step index 5 number of steps

To do curve fitting, we needed to have two C rates to compare with. With the data provided, we only have 0.5C, 1C, 2C, 3C and 5C. As such only 1C, 2C and 3C could be compared, as data existed for prior and forward C rates. We felt that this was a more accurate approach versus only picking two C rates rather than using 0.5C and 1C and do curve fitting with 3C and 5C with those. Again, we are using K1 at step index 5 to achieve this.

After picking the respective curves for the given C rate simulation, we imported them into the battery model using the following parameters. Note the NTGK parameter U and Y table manually had their temperatures adjusted to 25°C as highlighted below:

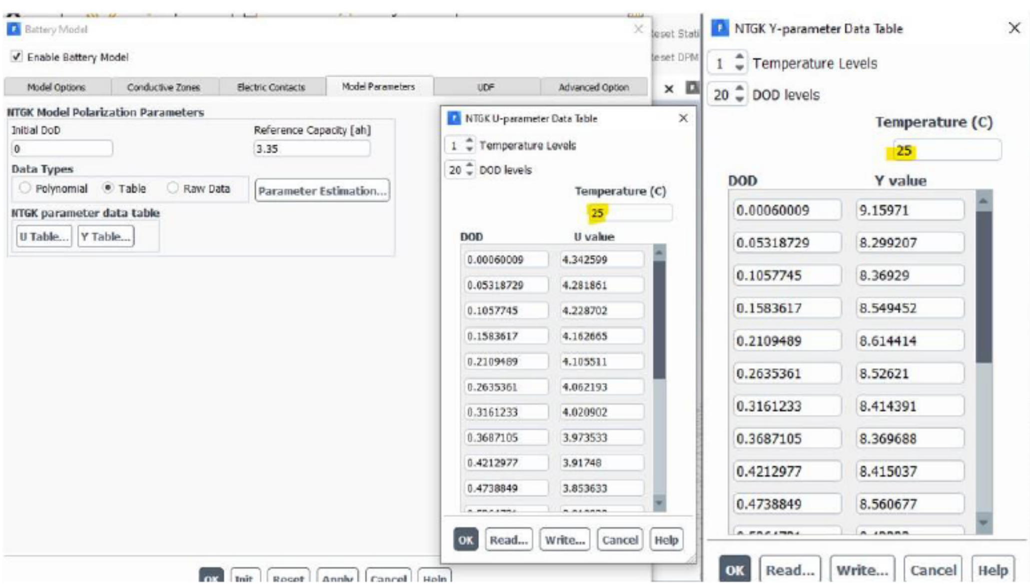


Figure 2.23 - Battery Curve Fitting Parameters

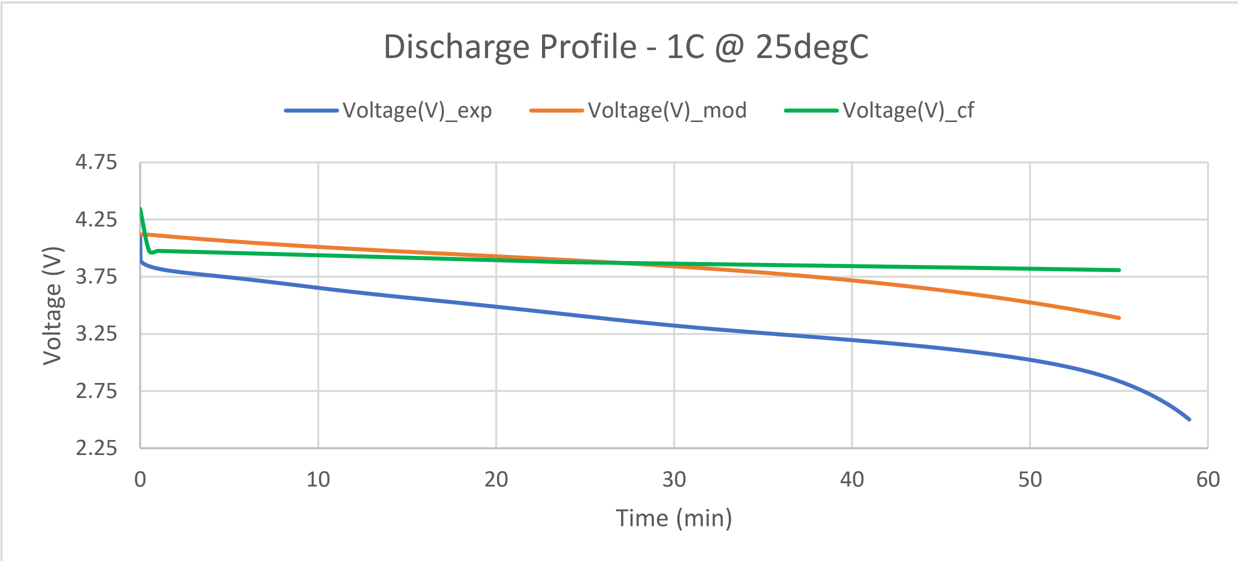


Figure 2.24 - Fitted Discharge Profile of 1C at 25°C

The figure above is identical to Figure 2.14 except that it has an added fit curve. When observed, we notice that it starts out at 4.3V and has a sudden drop to roughly 4V, which is a value that is in the middle of the other two curves. From there on, it decreases slightly in voltage towards the end at 55 mins. The change in voltage is approximately 0.2V.

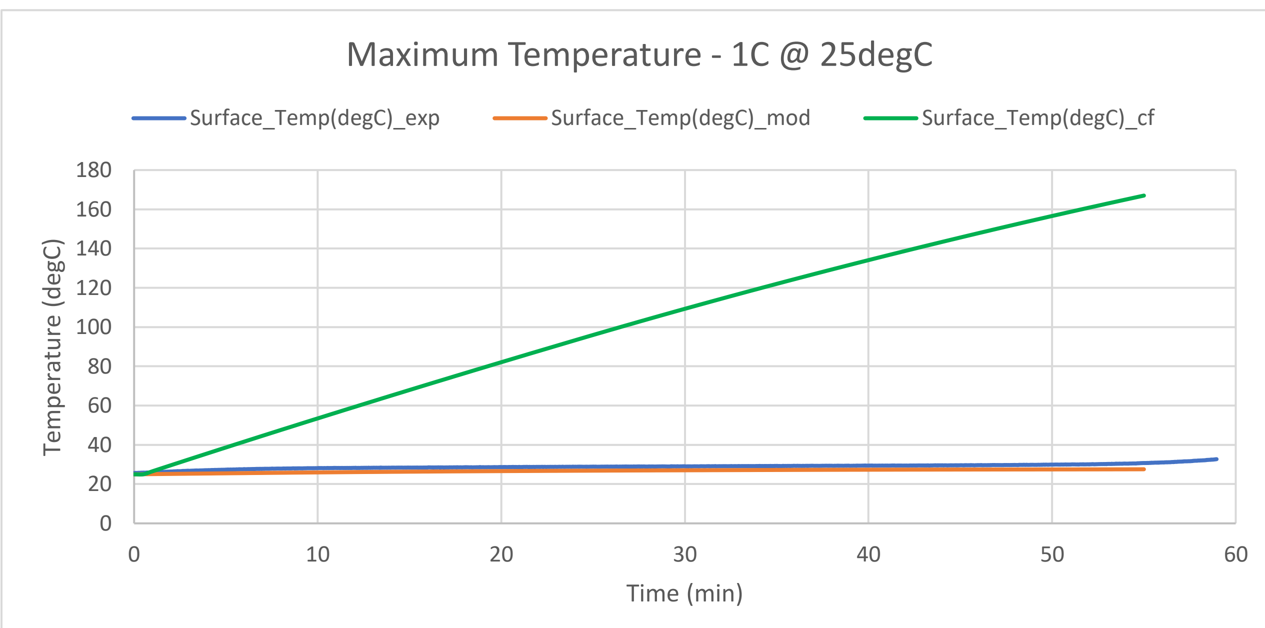


Figure 2.25 - Fitted Maximum Temperature of 1C at 25°C

The figure above is identical to Figure 2.15 except that it has an added fit curve. When observed, we notice that it does not quite resemble any similarity to our simulated and data provided curves.

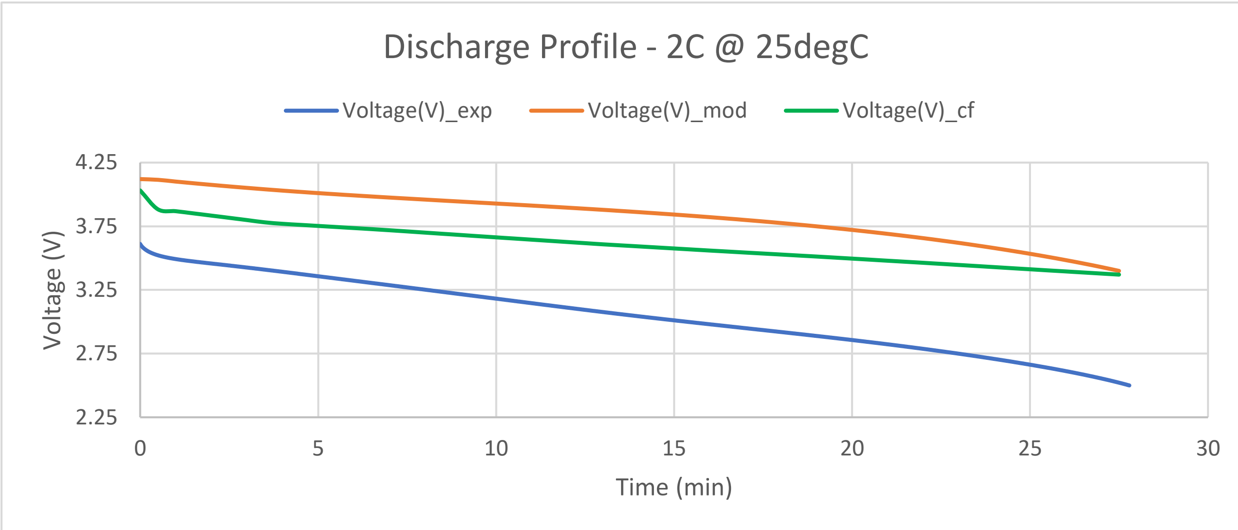


Figure 2.27 - Fitted Discharge Profile of 2C at 25°C

The figure above is identical to Figure 2.16 except that it has an added fit curve. When observed, we notice that the fitted curve is behaving as it should. It is closer to the Voltage(V)_exp curve, which is the data provided, and resembles a similar style. The fitted curve also begins and ends at approximately the same voltages.

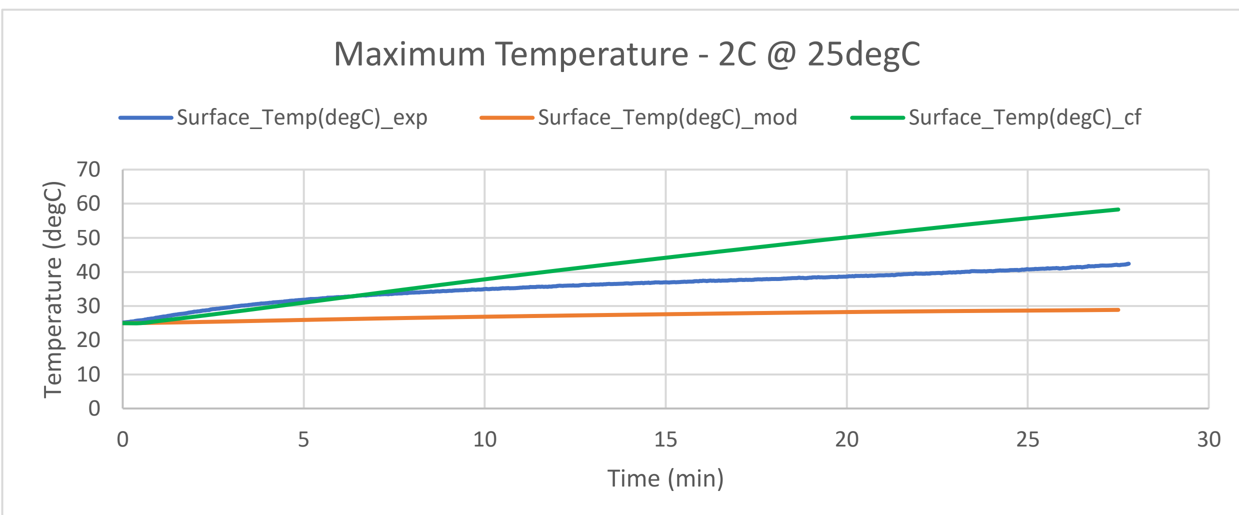


Figure 2.26 - Fitted Maximum Temperature of 2C at 25°C

The figure above is identical to Figure 2.17 except that it has an added fit curve. When observed, we notice that it does not quite fit accurately. The nature of a fit curve is to bring the simulated results closer to that of the data provided. In this case however, we see that it intercepts the data curve and peaks at a temperature that is almost 18°C higher.

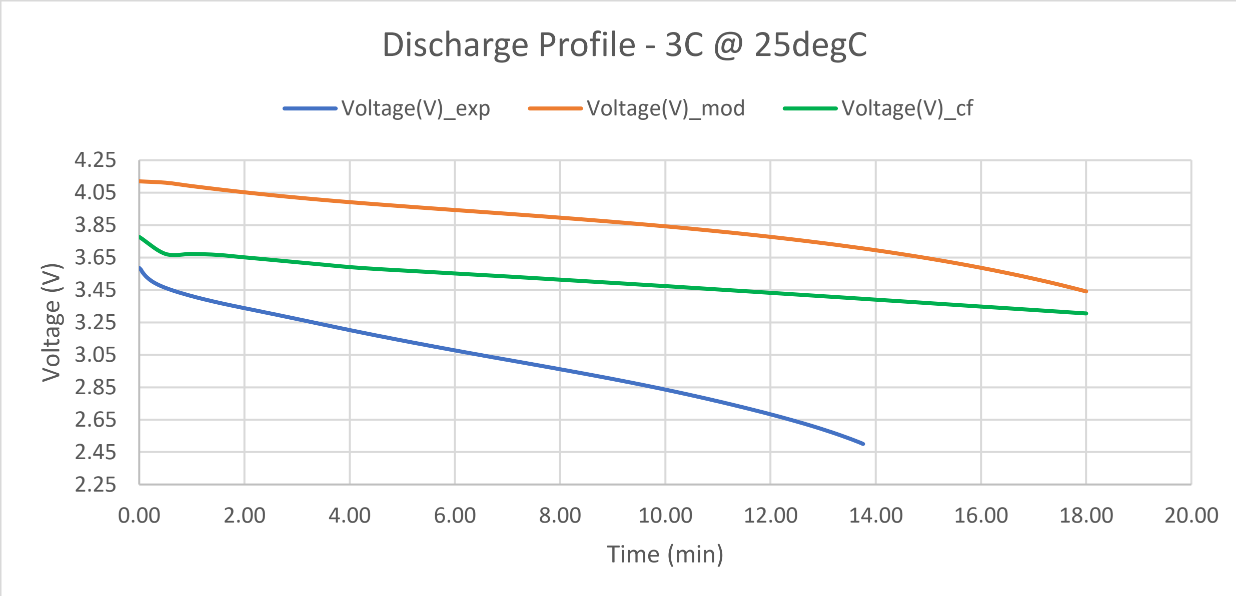


Figure 2.28 - Fitted Discharge Profile of 3C at 25°C.

The figure above is identical to Figure 2.18 except that it has an added fit curve. When observed, we notice that the fitted curve is behaving as it should. It is closer to the Voltage(V)_exp curve, which is the data provided, and resembles a similar style but a more positive slope. The fitted curve also tends to be approaching the same voltage to that of the simulated (Voltage(V)_mod) curve.

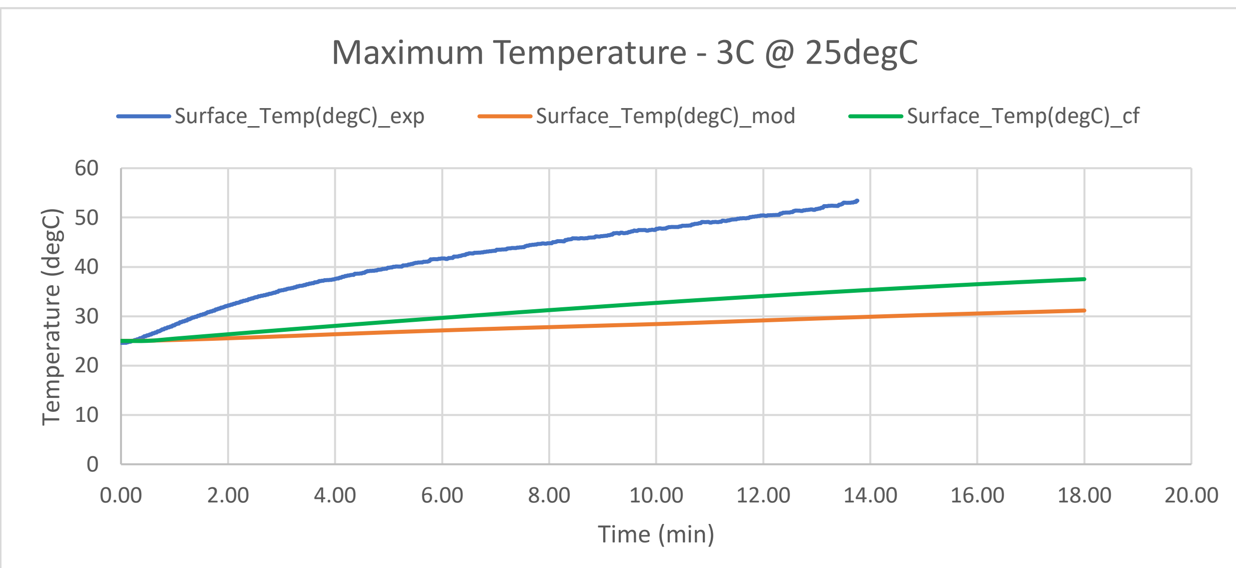


Figure 2.29 - Fitted Maximum Temperature of 3C at 25°C

The figure above is identical to Figure 2.19 except that it has an added fit curve. When observed, we notice that it does fit accurately. The nature of a fit curve is to bring the simulated results closer to that of the data provided. In this case we see this happening and what was originally simulated to be a max peak temp of 31°C is now 38°C, and 7°C more closer to the peak of the data provided (54°C).

Part 3- Cylindrical Battery Comparison Challenge: 4C Discharge Rate at Different Temperatures

The next challenge is to use the cylindrical battery model to analyze results from scenarios in which we did not have experimental data. The model has been validated regarding the rectangular battery with the tutorial results, and the cylindrical battery experimental data for 1C, 2C, 3C and 5C at 25 ^{O}C. It was shown that we produce accurate data, so it is ensured that the results regarding different C-rates or ambient/starting temperatures will be accurate. The model was analyzed at 4C with starting battery temperatures of 0, 25, and 50 ^{O}C. To set up the correct run time for the 4C discharge rate, the run calculations parameters, including time step size [min] and no. of time steps, are shown in Figure 3.1. The model was run for 14min, which can be seen in the figure below.

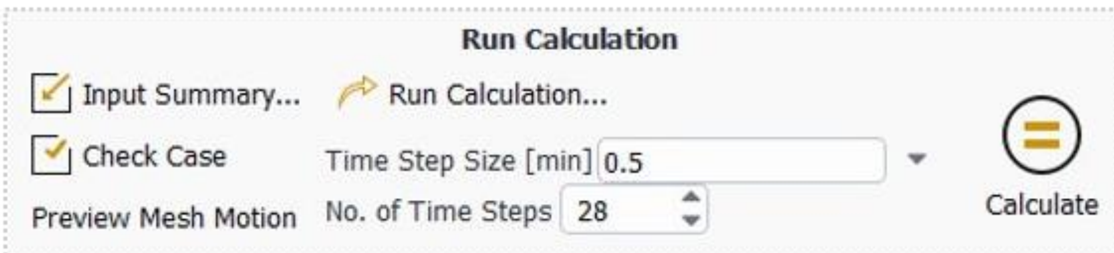


Figure 3.1 - Run Calculation parameters used for all runs at 4C rate for a total of 14 min. run time

For the results and discussion, first the cathode and anode potentials will be compared at the different temperatures. Then, the three different discharge curve results from our simulations will be discussed. Next, the maximum temperature contour plots are analyzed along with the max temperature curves over the time that the battery is discharged. To conclude the 4C results, the combined data for all three temperatures are shown for discussion. Finally, the discharge curves and temperature versus time plots of the five C-rates at 25 ^{O}C are compiled together as a complete review.

When comparing the cathode and anode potentials for the 4C rate, similar results and trends were found from that of the 1C, 2C, 3C, and 5C. Figures 3.2, 3.3, and 3.4 represent the potential contour plots for 0, 25, and 50 ^{O}C, respectively. From the plots, it can be concluded that the temperature does not affect the dispersion of the potential at the tabs. This is for only small temperature changes; if extreme temperature changes were applied, there is a possibility we see more of a difference. However, for our temperature range (0 – 50 ^{O}C) there is not a change in anode and cathode potential dispersion in the cylindrical battery model. The contours are shown on the next page.

Cathode and Anode Comparisons at Different Ambient Temperature

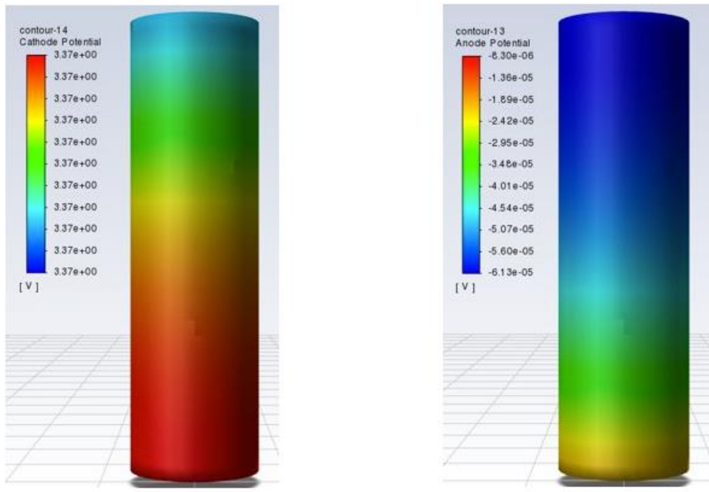


Figure 3.2 – Cathode (left) and Anode (right) at 4C discharge rate at starting temperature of 0°C.

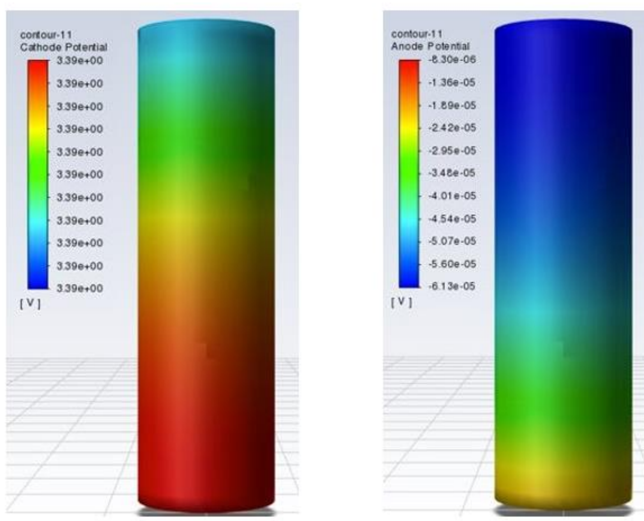


Figure 3.3 – Cathode (left) and Anode (right) at 4C discharge rate at starting temperature of 25°C.

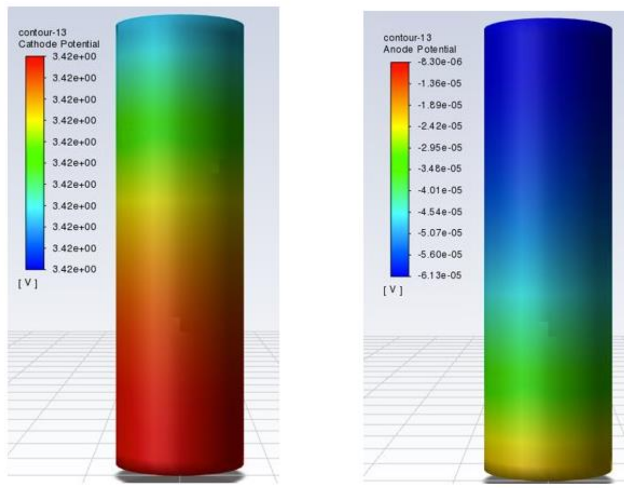


Figure 3.4 – Cathode (left) and Anode (right) at 4C discharge rate at starting temperature of 50°C.

For the maximum temperature, contour plots can show the temperature dispersion throughout the battery. Figure 3.5 shows the contour plots of maximum temperature for all three starting temperatures for the 4C rate. The higher the starting the temperature, the higher the maximum temperature in the battery is. It is important to notice the dispersion of the temperature. It is shown that as the starting temperature increases, more of the battery reaches the maximum temperature, especially through the cathode. At more extreme high temperatures, it can be hypothesized that the entire cylindrical battery can reach the maximum temperature, in turn creating more concern for heat transfer management in the battery module or pack. This contour is available below.

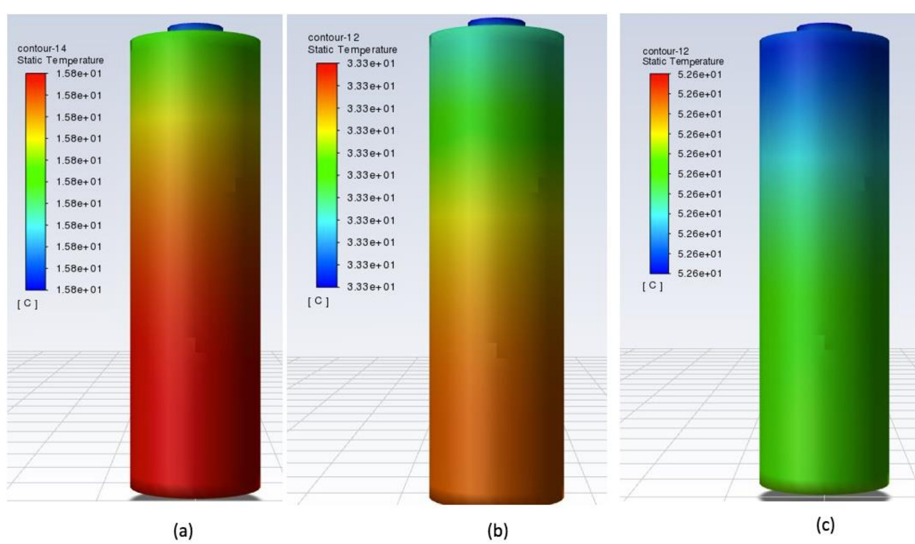


Figure 3.5 – Maximum temperature contour plots at discharge of 4C for starting temperatures of (a) 0, (b) 25, and (c) 50°C

Comparison of ANSYS Raw Data

Charting of the raw data from ANSYS (including discharge profile and maximum temperature over time) is shown in Figures 3.6, 3.7 and 3.8 for 0, 25, and 50 ^{O}C, respectively. From a quick view, the voltage discharge profiles are similar and discharge to the same voltage. The temperature profiles show that the batteries all start at different temperatures (in alliance with what we set in our model) and the slopes and end maximum temperatures are all different. These comparisons between different starting temperatures are discussed next and will allow of a better discussion.

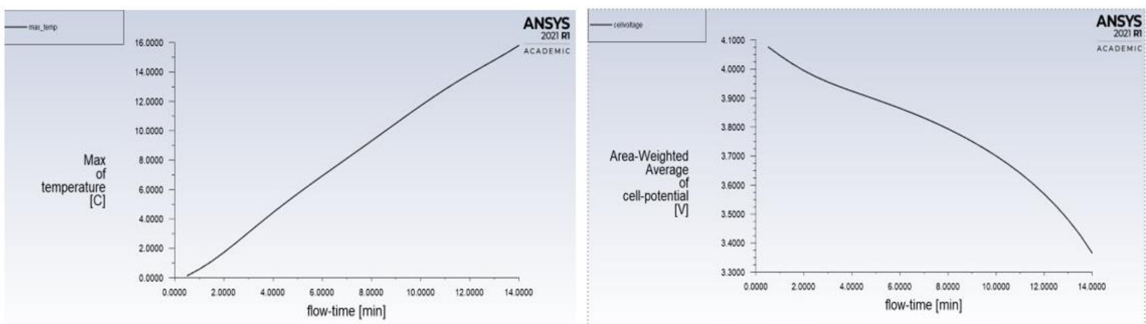


Figure 3.6 – ANSYS data of maximum temperature (left) and discharge profile (right) for 4C @ 0°C.

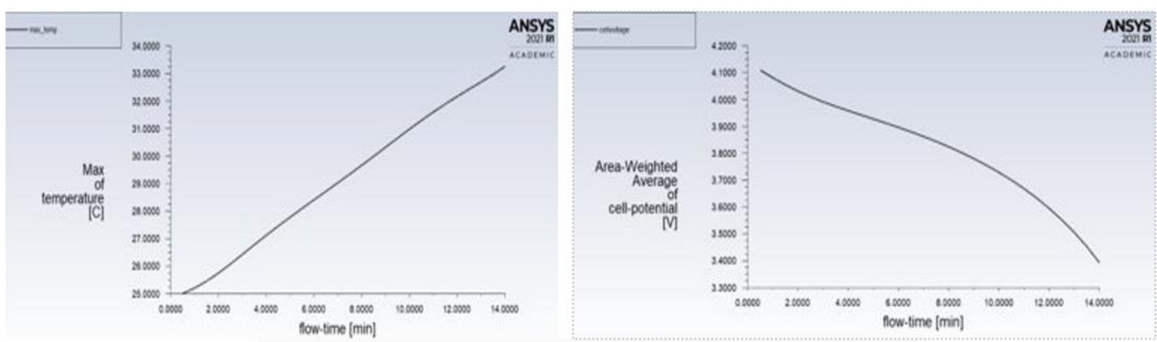


Figure 3.7 – ANSYS data of maximum temperature (left) and discharge profile (right) for 4C @ 25°C.

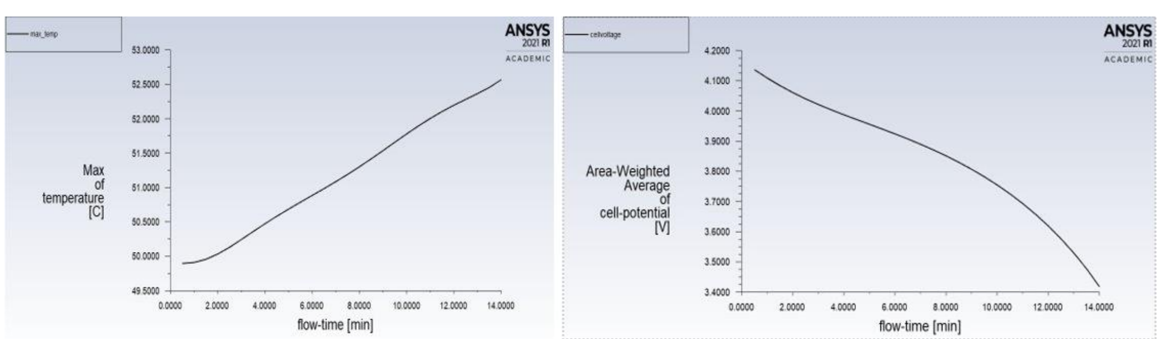


Figure 3.8 – ANSYS data of maximum temperature (left) and discharge profile (right) for 4C @ 50°C.

Comparison of all Discharge Rate Simulations

The discharge profiles for all three starting temperatures for the 4C rate that was ran in the model are shown together in Figure 3.9, below. At first glance, the results look similar but there are three points to be noticed here. First, the starting voltage drops initially as the temperature decreases. This shows that the colder the temperature the battery is operating in, the less voltage you can get out of the battery. Next, we can notice that the slopes are relatively the same, except in one area for the 0 ^{O}C where an initial dip in voltage occurs at the beginning of the discharge. Finally, it is important to point out that at extreme temperatures, high or low, these trends we noticed would be more drastic. While we measured the data at reasonable starting temperatures, in a very hot or cold climate, one may have to consider that the total voltage we may obtain from the battery and the way it discharges may be different.

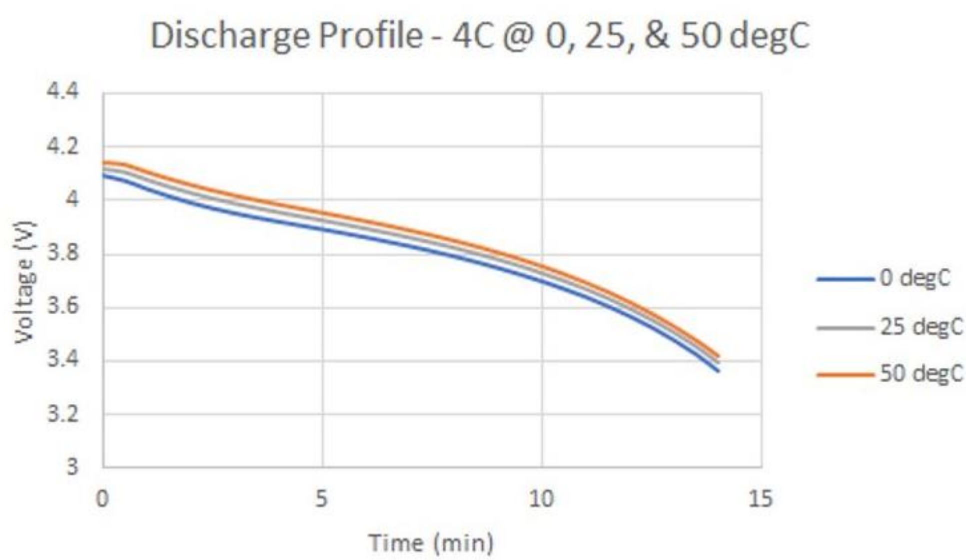


Figure 3.9 – Discharge profile of all three starting temperatures for 4C rate.

The next comparison that will be discussed is the change in maximum temperature over time for each starting temperature at the 4C rate (Figure 3.10.) There are a couple of observations to discuss from this chart. It is obvious that we see the plots starting at different temperatures and, it is shown that they start at the correct temperatures that were expected, based on the starting temperatures set in the model. As time goes on and the battery begins to discharge, we see a difference in temperature for each case. The slope for each set of data is different. This goes on to let us conclude that the colder the starting temperature is, the higher increase in total temperature is seen. For the high temperatures, the overall change in temperature is not as much, but it still reaches the highest maximum temperature, which would be the main concern when examining the battery module/pack for heat transfer problems to the system.

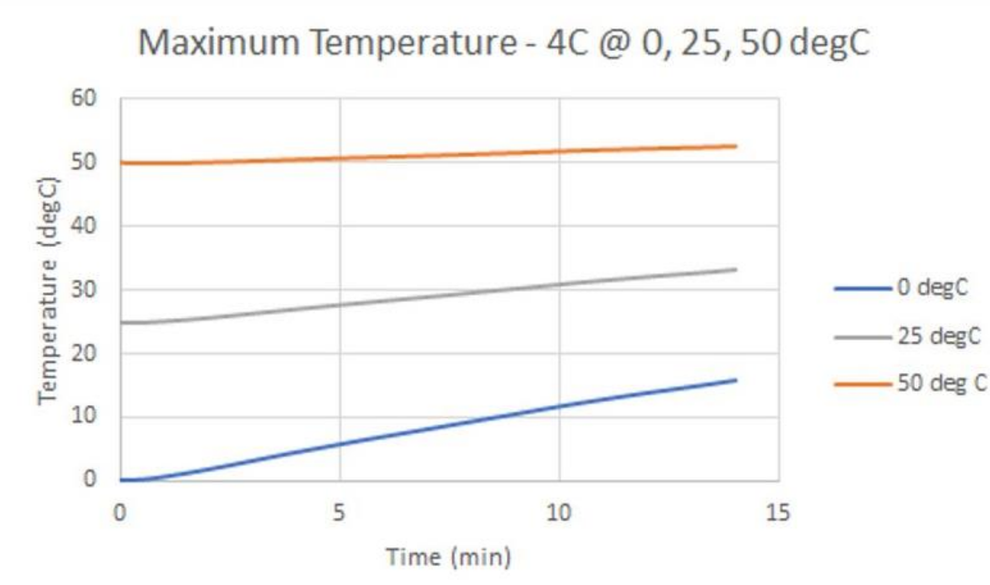


Figure 3.10 – Maximum temperature versus time for all three starting temperatures at 4C rate.

Finally, the comparison of all C-rates (1C, 2C, 3C, 4C, and 5C) is conducted at 25 ^{O}C to discuss any trends. The discharge curves, as shown in Figure 3.11, show that as the C-rate increases from 1 to 5, the total time of discharge decreases. This is as expected, and the results accurately depict those assumptions. Even though they run for different total times, all simulations discharge to the same voltage at the end of the analysis. Additionally, the maximum temperature over time was plotted for each C-rate for comparison in Figure 3.12. As expected, each simulation began at 25 ^{O}C and increase as time goes on. Like the discharge profiles, they reach maximum temperatures quicker as the C-rate increases. Also, the higher the C-rate, the quicker the temperature rises and the maximum temperature at the end of discharge gets exponentially higher as the C-rate increases from 1 to 5. For lower C-rates, the temperature increase starts to slow down as the battery reaches complete discharge. In contrast, for the 5C rate, there is an almost linear trend of temperature increase. For both the discharge profile and maximum temperatures, the 4C data ran in the model fits the trends of the other C-rates which were validated by experimental data. Figures are available on the next page.

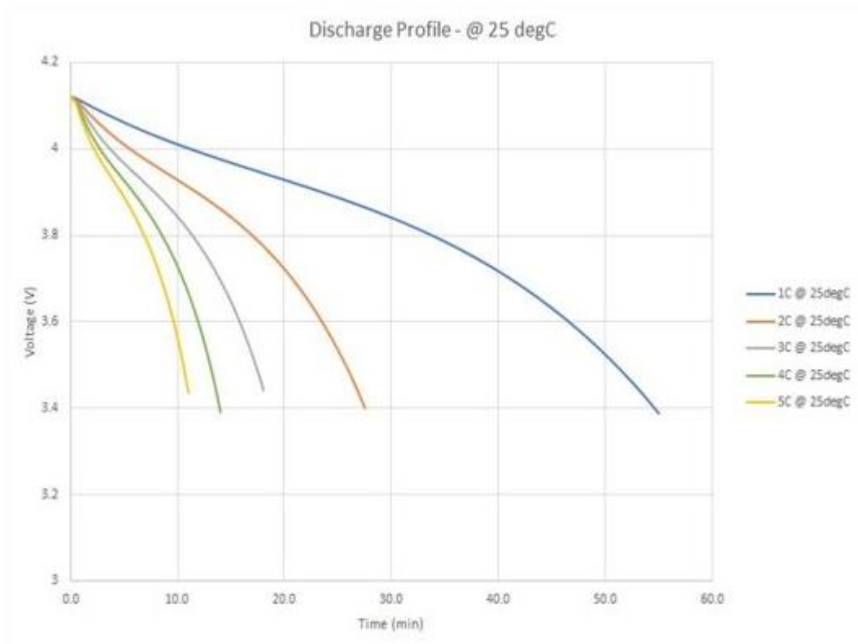


Figure 3.11 – Discharge profile for comparing multiple C-rates (1-5) at the same starting temperature (25°C).

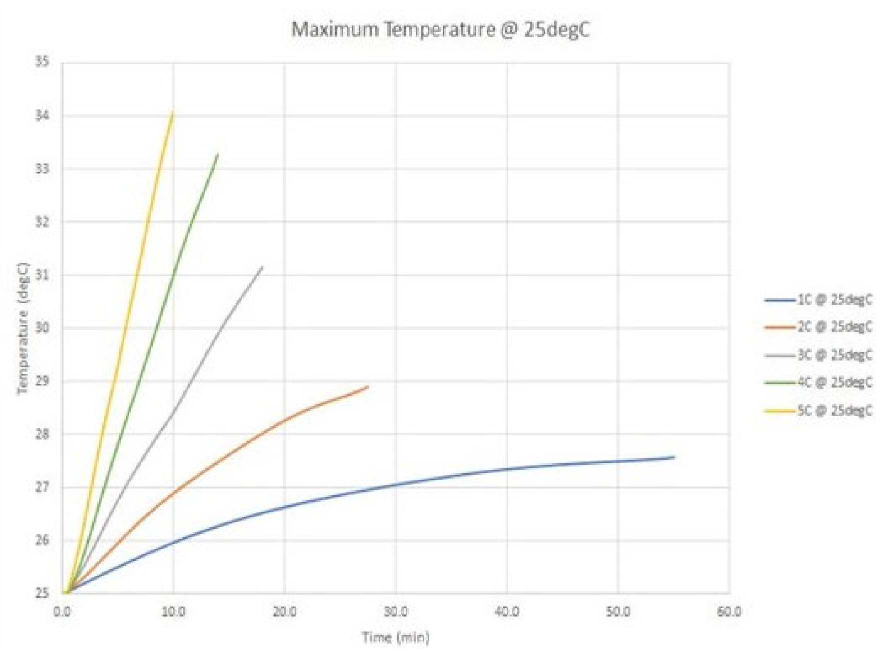


Figure 3.12 – Maximum temperature versus time for comparing multiple C-rates (1-5) at the same starting temperature (25°C).

Conclusions

Through this simulation project, our team learnt to use the ANSYS Fluent software and were able to use that knowledge to replicate the tutorial given in class, as well as a research paper. We showed that we were able to successfully replicate the tutorial, using contours and graphs to prove that our simulation was set up correctly, and provided evidence that our results matched with the tutorial simulation data. We were also able to replicate some results from a research paper, showing discharge rates at 1C, 2C, 3C, and 5C. We had to develop our own cylindrical battery model and mesh to run these simulations ourselves. We were then challenged to run the same simulation at 4C, and to investigate the affect of ambient temperature of discharge at that rate. We investigated discharge at ambient temperatures of 0,25, and 50 ^{O}C. We also plotted all discharge and temperature profiles for every discharge rate, at an ambient temperature of 25 ^{O}C. We can conclude that higher discharge rates induce higher operating temperatures of the battery cell, and that as the temperature drops, the total charge that one can get out of a battery cell is reduced. These effects would be much more noticeable in extreme temperatures.

This project required knowledge of battery cell systems, and the ability to use ANSYS Fluent to run battery simulations. Through this project, we simulated rectangular and cylindrical battery cells, and were able to run simulations on both types of batteries without crashes. Our data was consistent with our expectations based on discharge rates and temperature, so we feel confident that our simulations were run correctly. This project required our team to learn new skills while implementing knowledge gained through classwork and was a good practical use of the information and concepts that we learned in the classroom.

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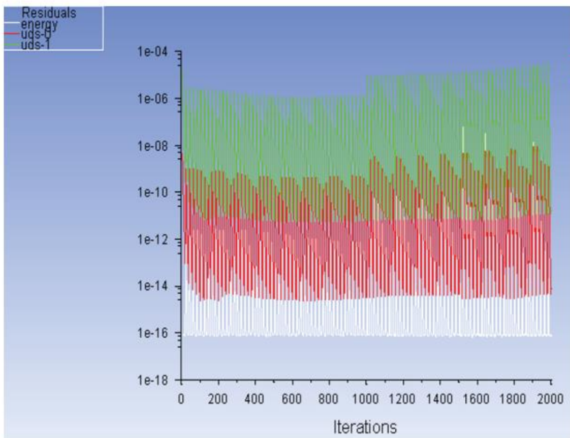
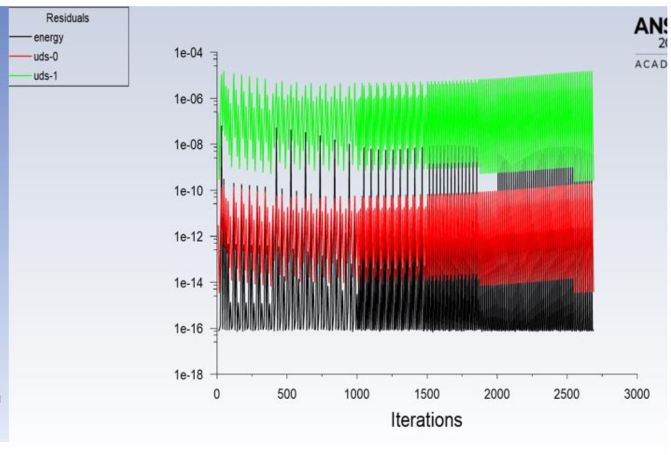
Appendix A

All Figures and Plots for Part 1

1C - Residual History
Tutorial vs Simulation

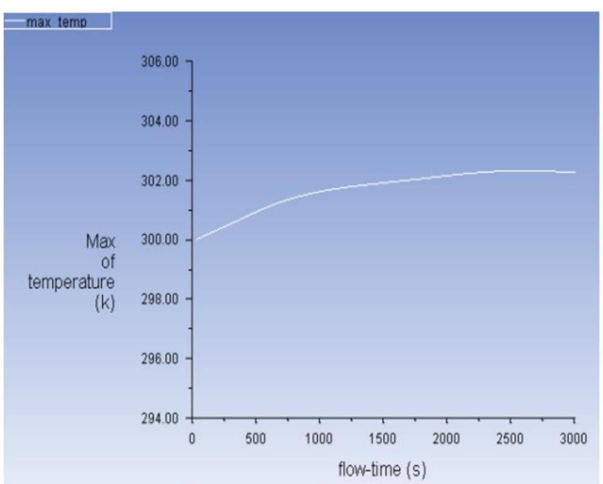


Tutorial

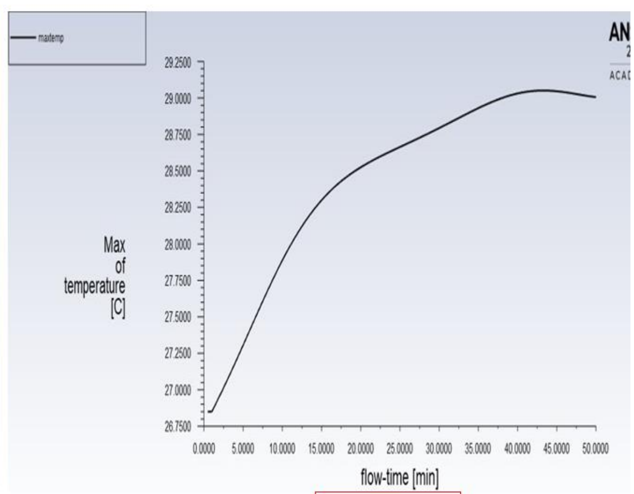


Simulation

1C – Temperature Curve
Tutorial vs Simulation

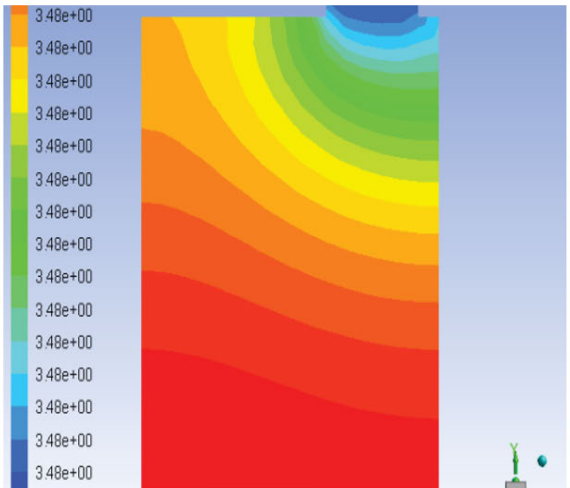


Tutorial

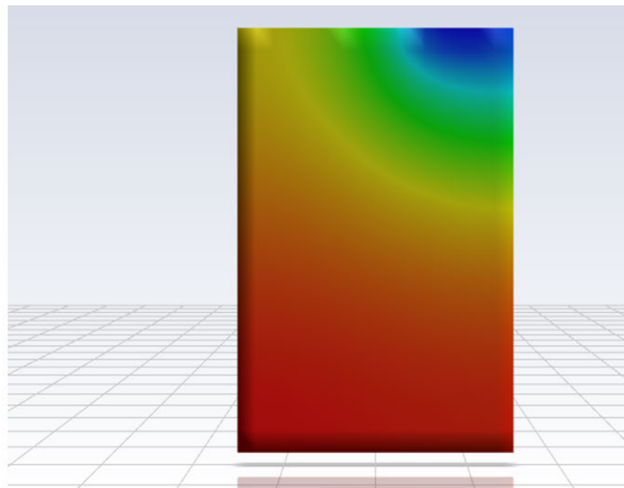


Simulation

1C – Cathode Potential Tutorial vs Simulation

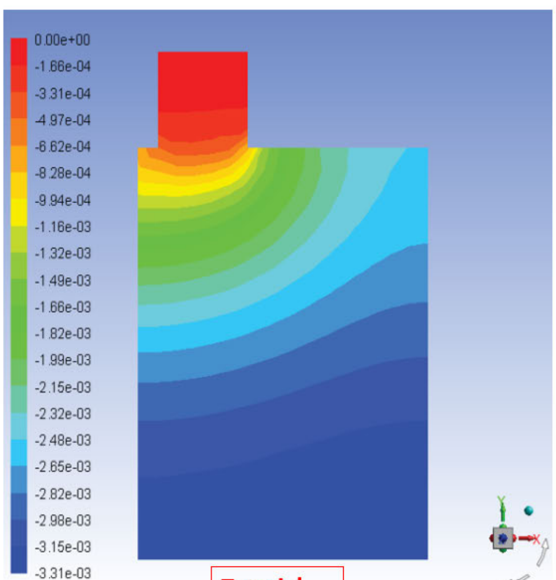


Tutorial

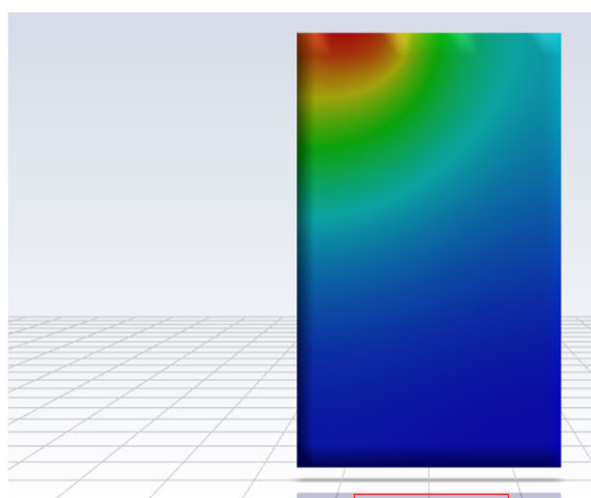


Simulation

1C – Anode Potential Tutorial vs Simulation

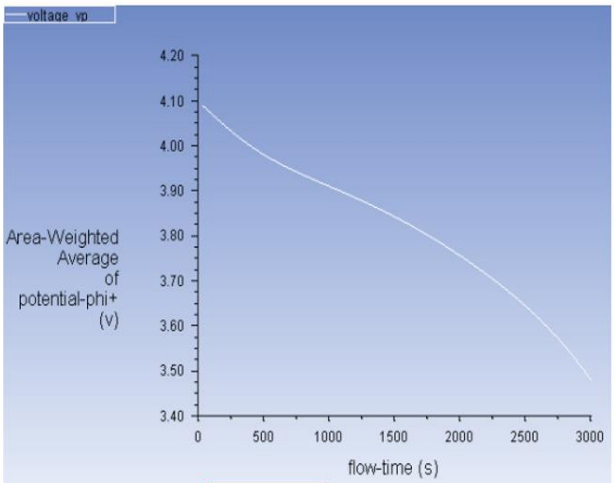


Tutorial

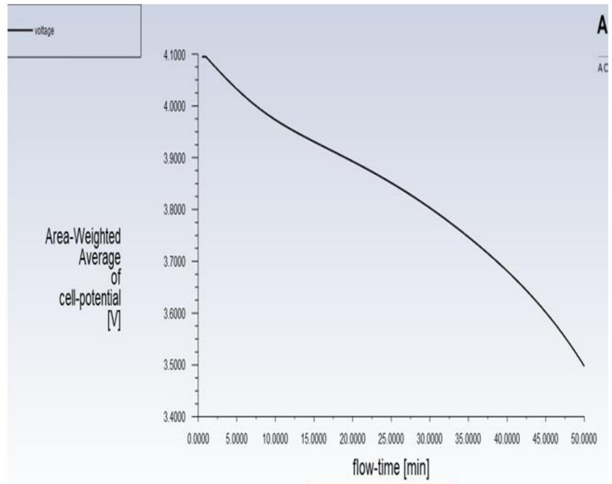


Simulation

1C – Voltage Curve Tutorial vs Simulation

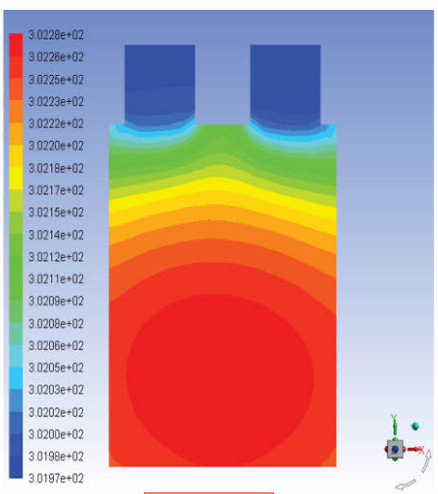


Tutorial

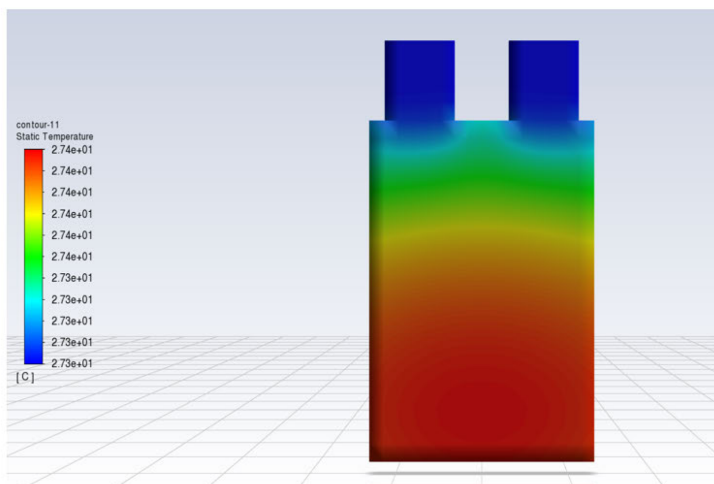


Simulation

1C - Contour Plot of Temperature Tutorial vs Simulation



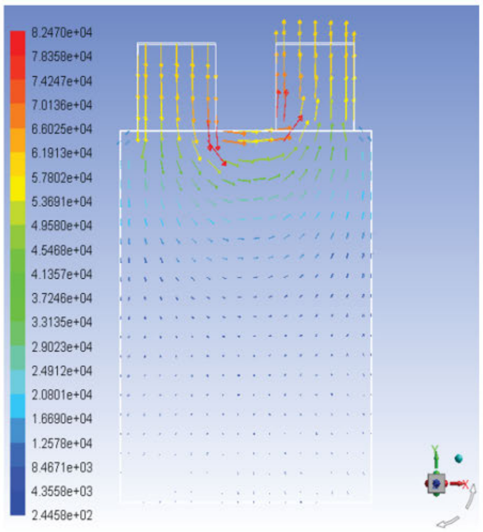
Tutorial



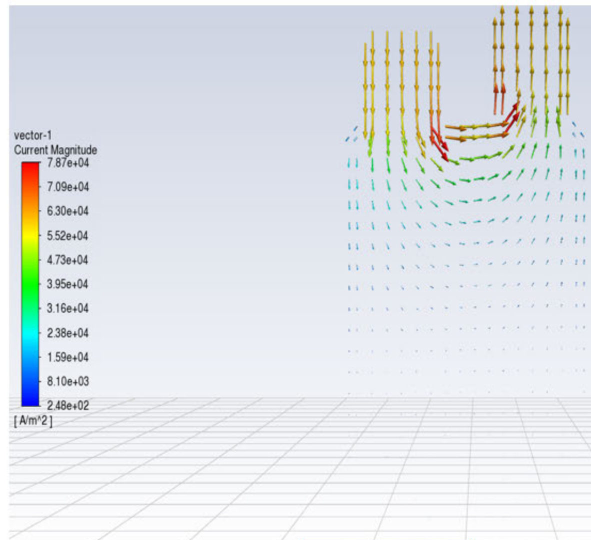
Simulation

13

1C - Vector Plot of Current Density Tutorial vs Simulation

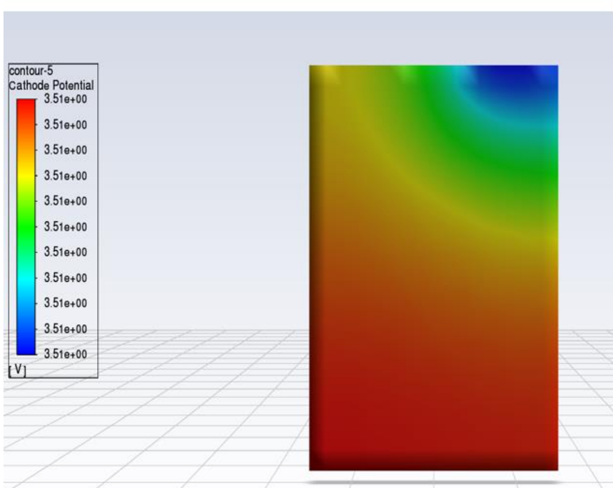


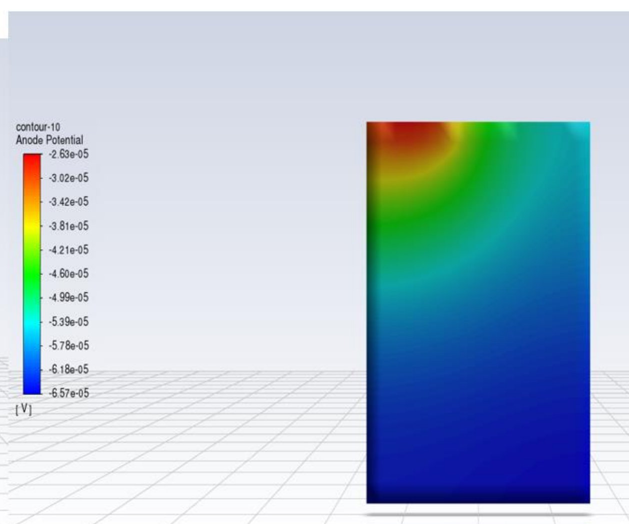
Tutorial



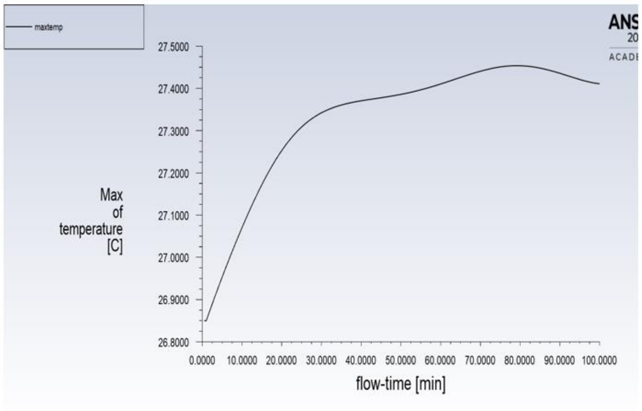
Simulation

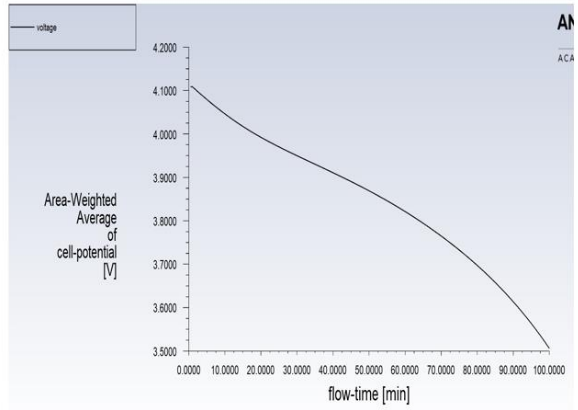
0.5C – Cathode & Anode Potential



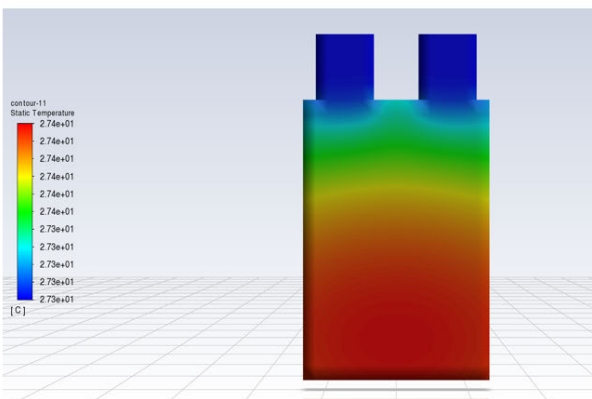


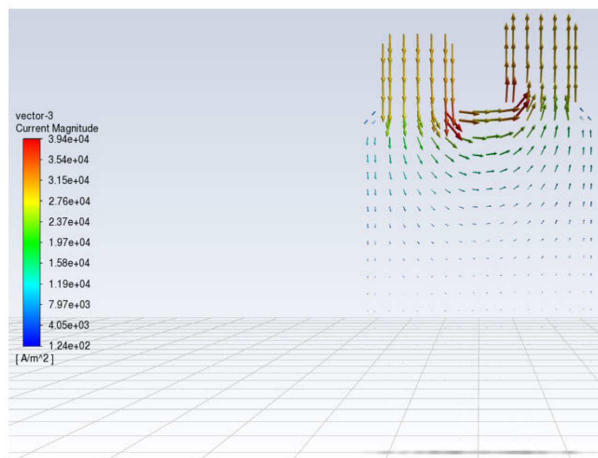
0.5C – Temperature & Voltage Curves



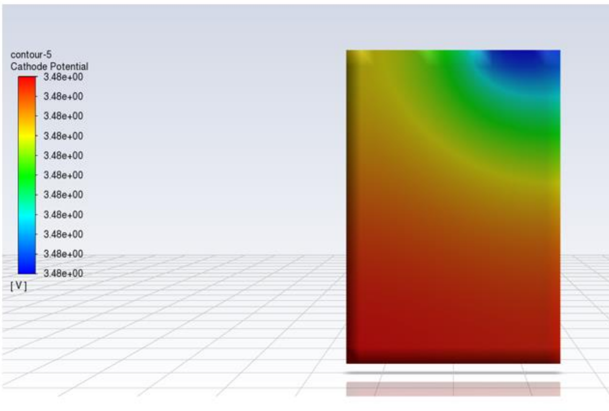


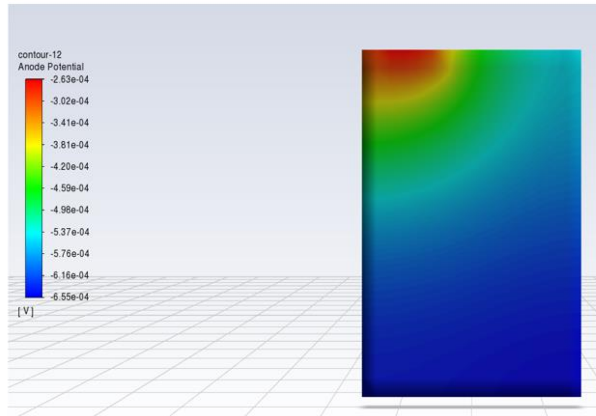
0.5C - Contour of Temperature & Vector Plot of Current Density



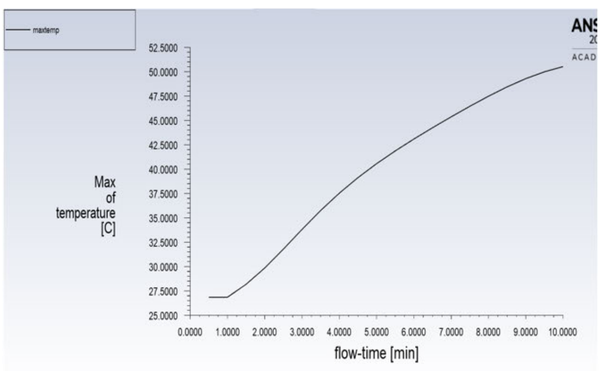


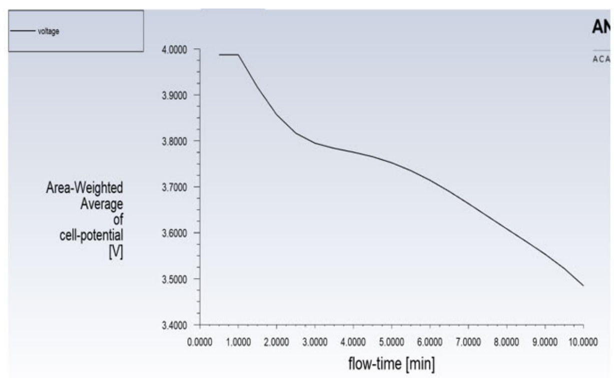
5C – Cathode & Anode Potential



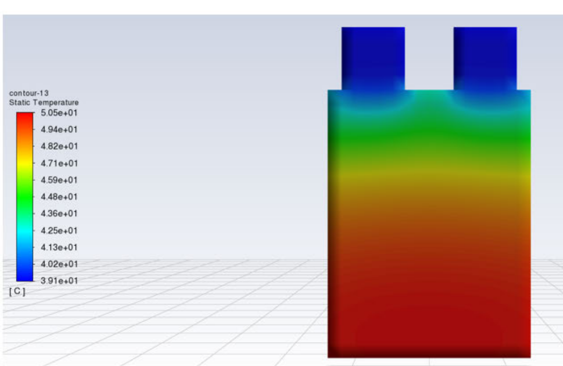


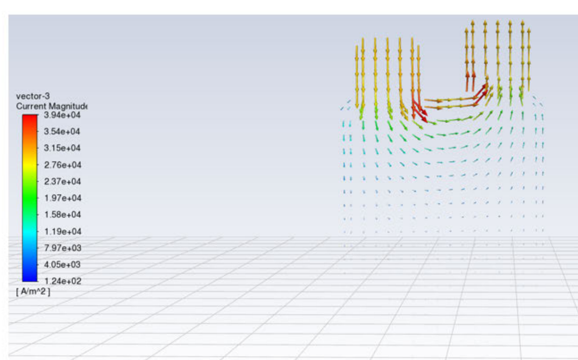
5C – Temperature & Voltage Curve





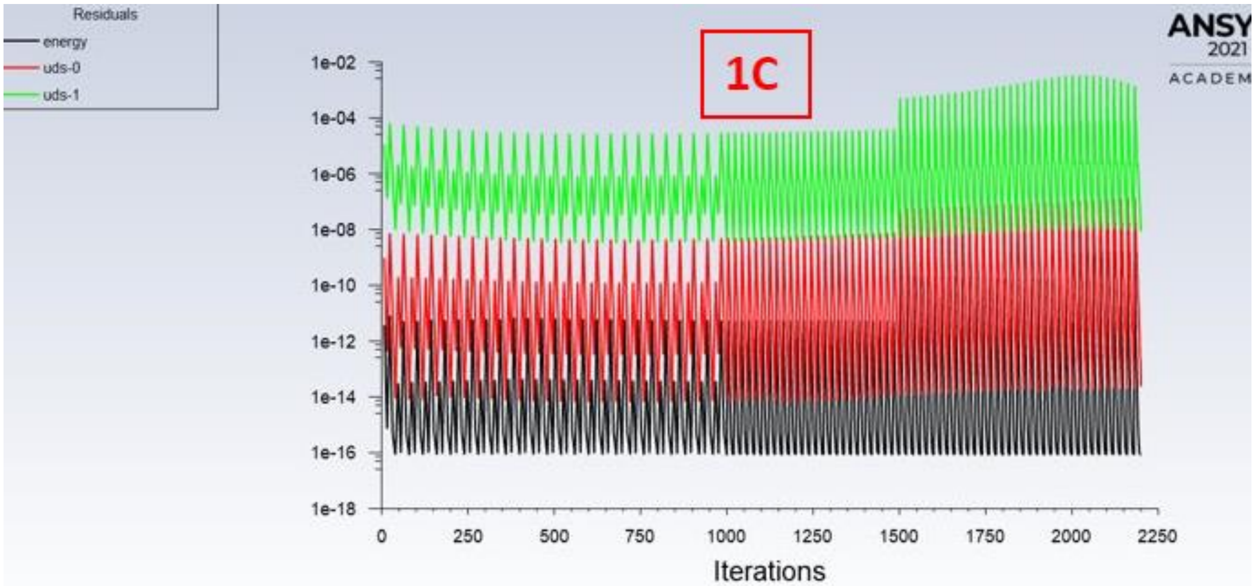
5C - Contour of Temperature & Vector Plot of Current Density

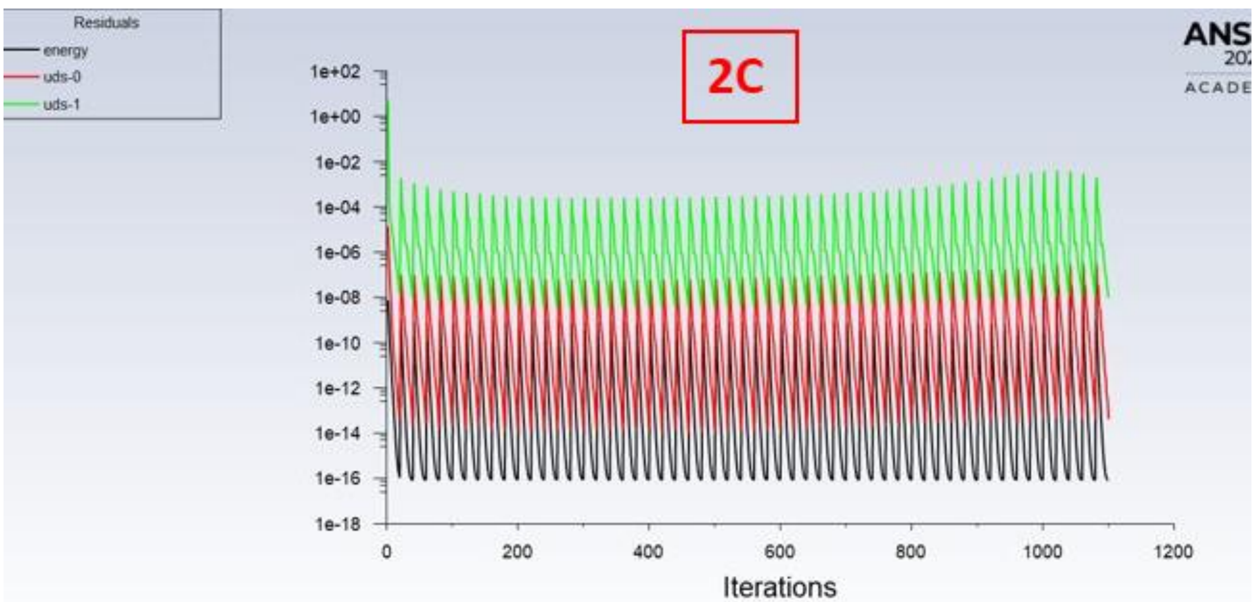


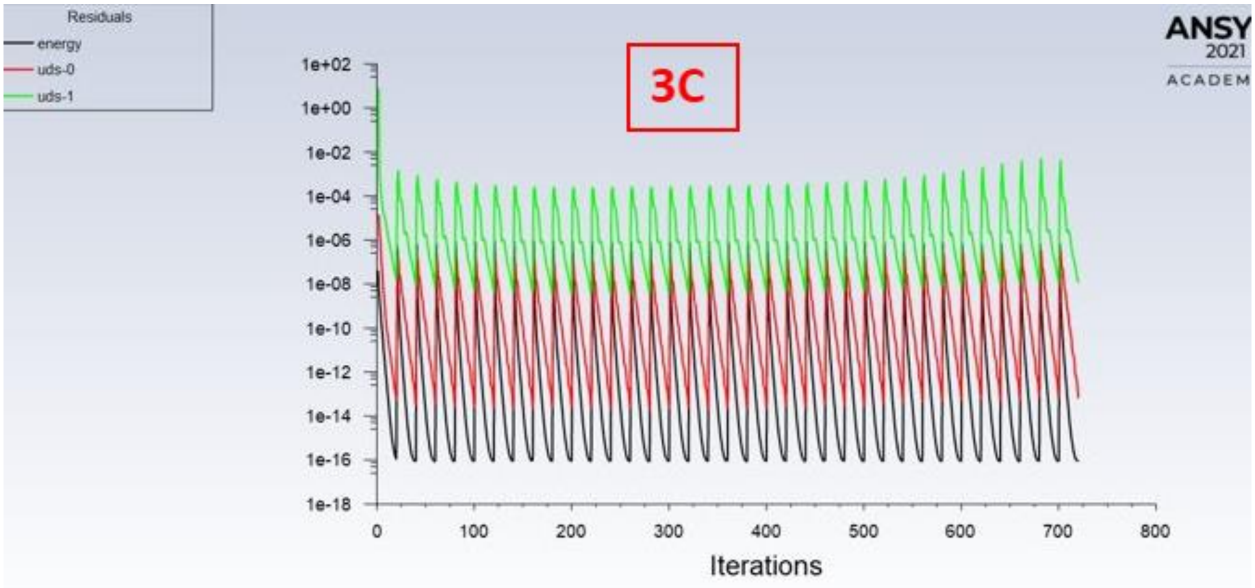


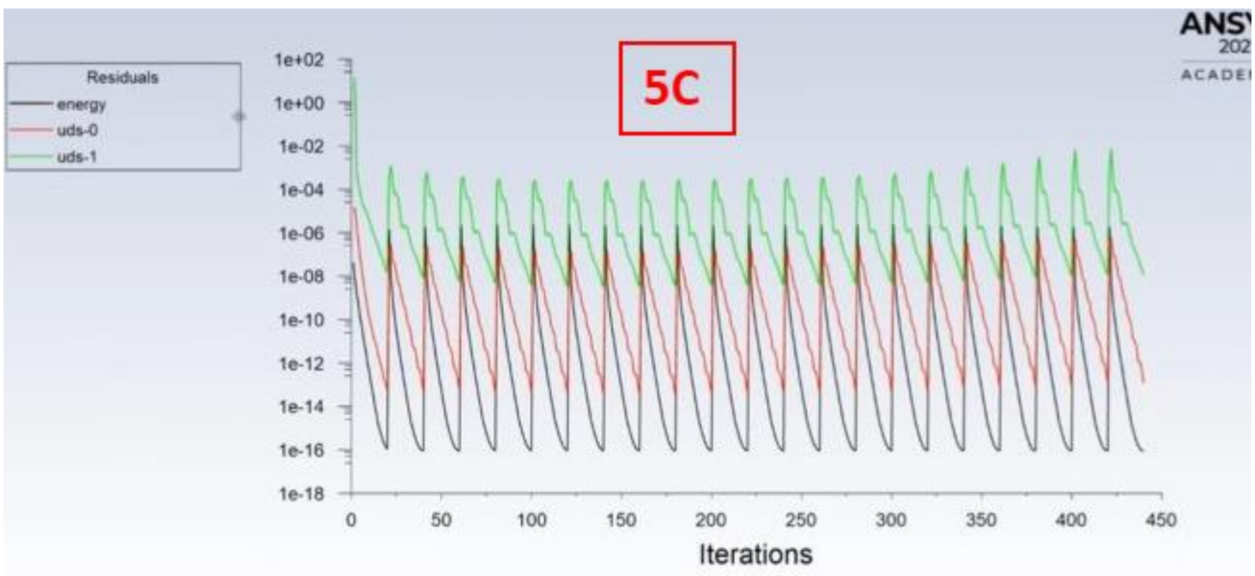
All Figures and Plots for Part 2

Scaled Residuals for 1C, 2C, 3C and 5C for cylindrical cell battery

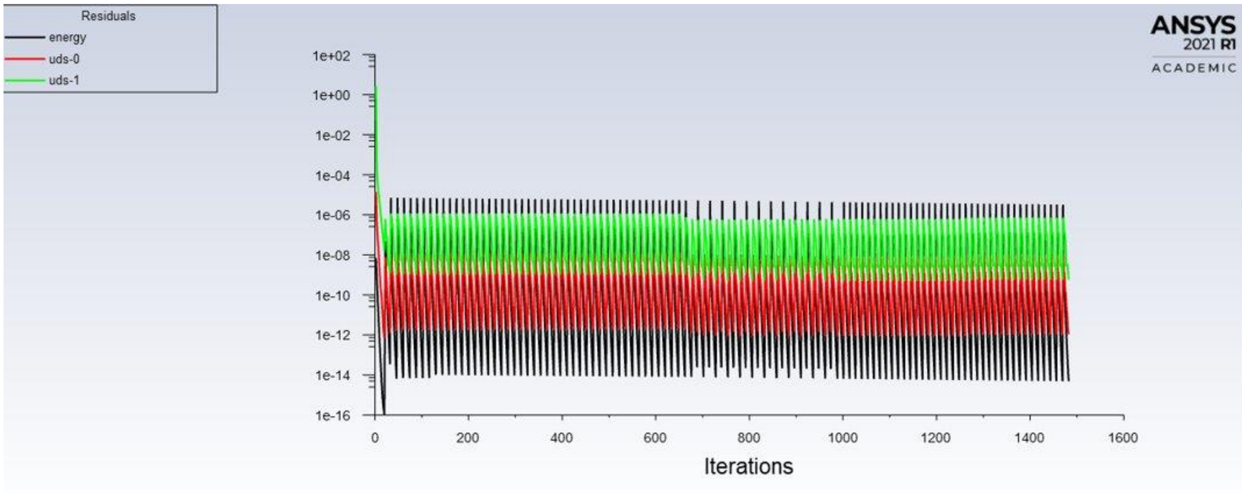


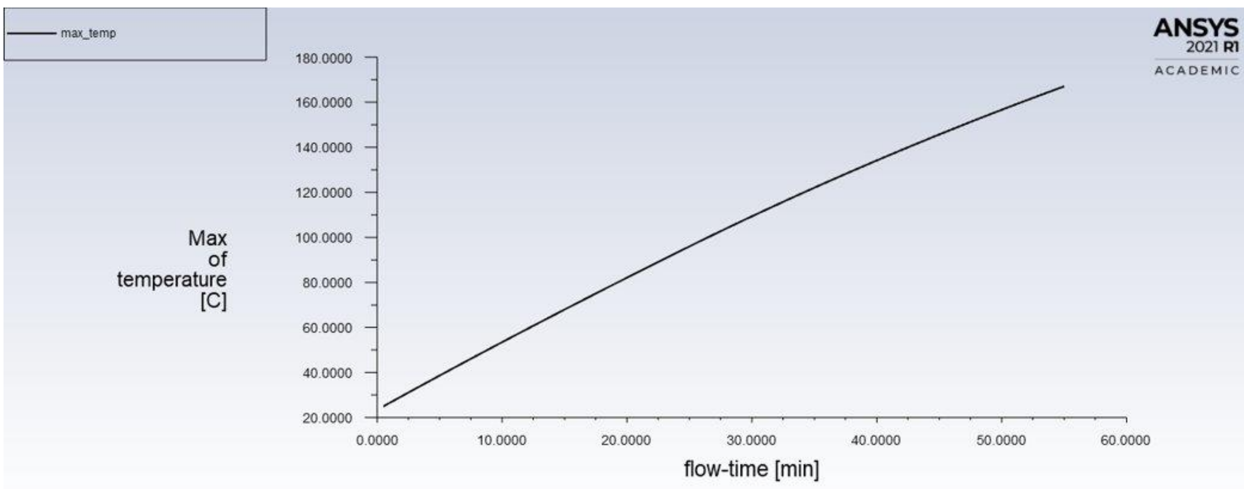


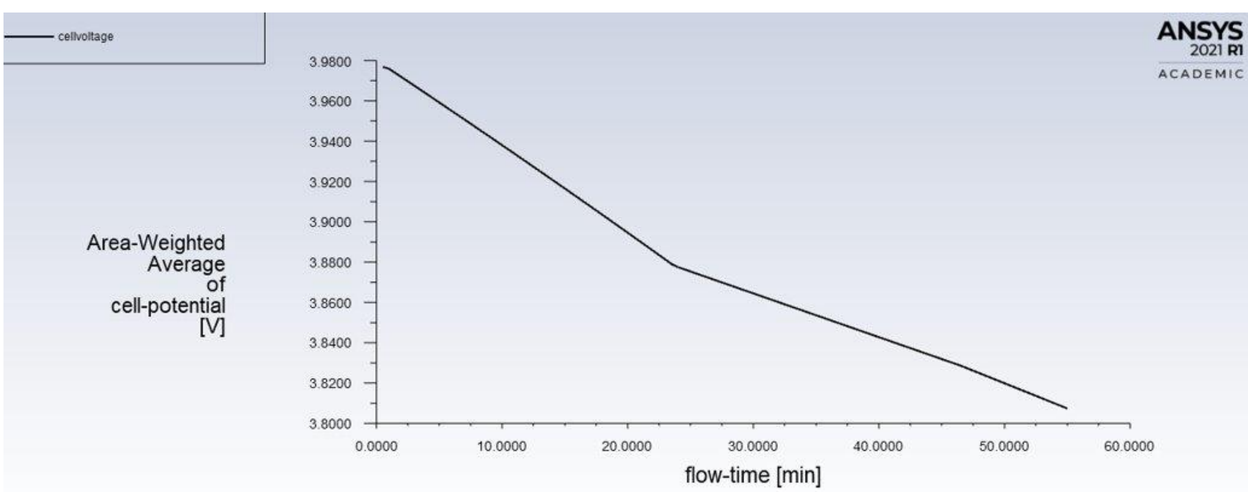

Residuals
energy
uds-0
uds-1
3C
ANSY
2021
ACADEM
1e+02
1e+00
1e-02
1e-04
1e-06
1e-08
1e-10
1e-12
1e-14
1e-16
1e-18
0
100
200
300
400
500
600
700
800
Iterations

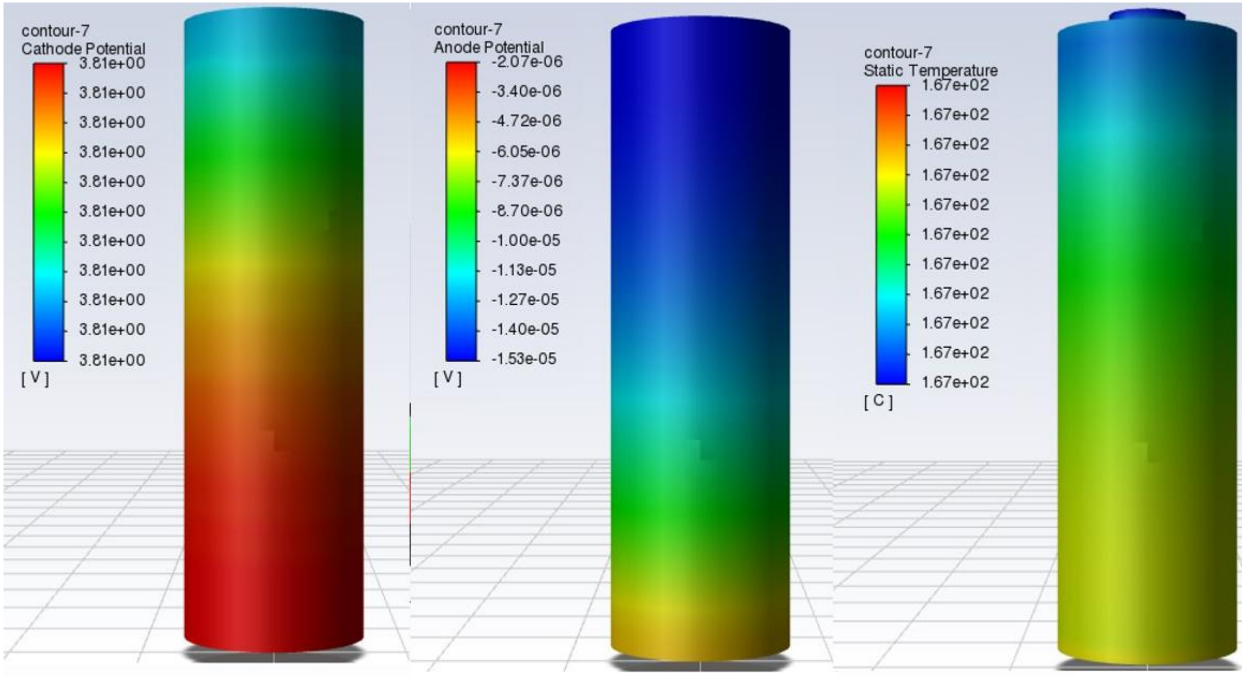

Residuals
energy
uds-0
uds-1
5C
ANSY
202
ACADE
1e+02
1e+00
1e-02
1e-04
1e-06
1e-08
1e-10
1e-12
1e-14
1e-16
1e-18
0
50
100
150
200
250
300
350
400
450
Iterations

1C after fitting with 0.5C and 2C raw data:

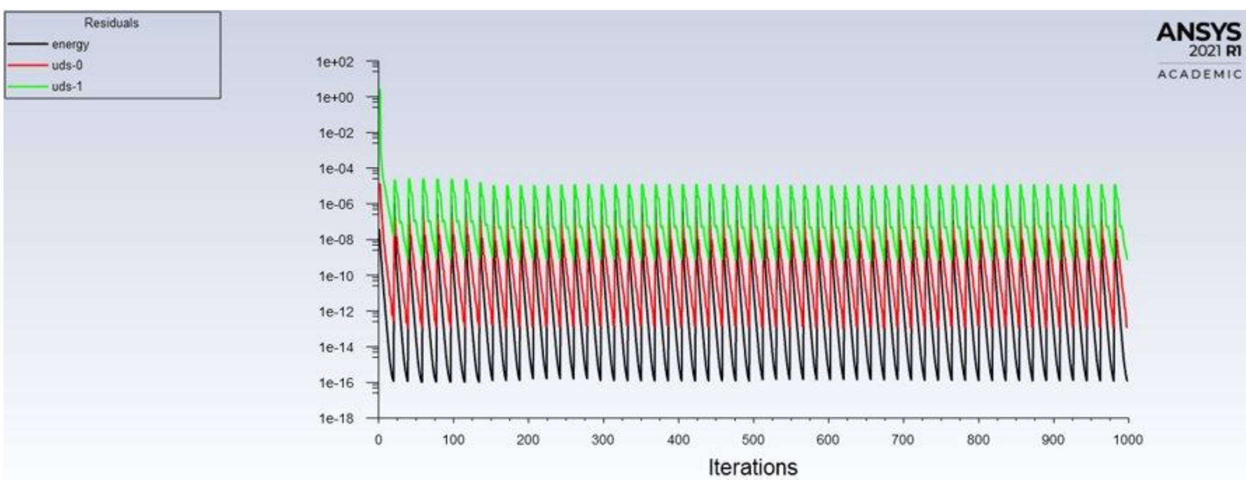


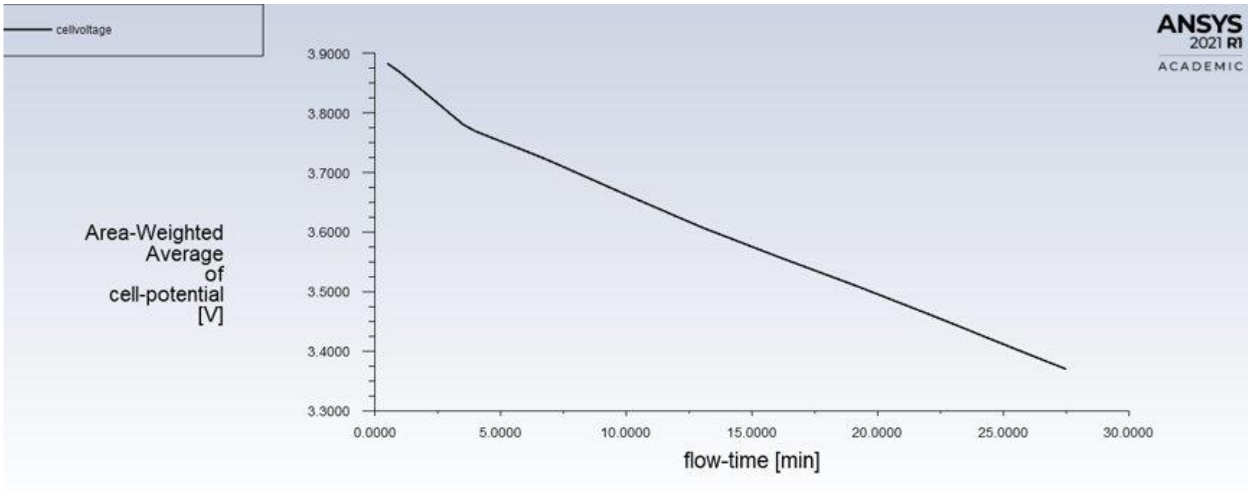


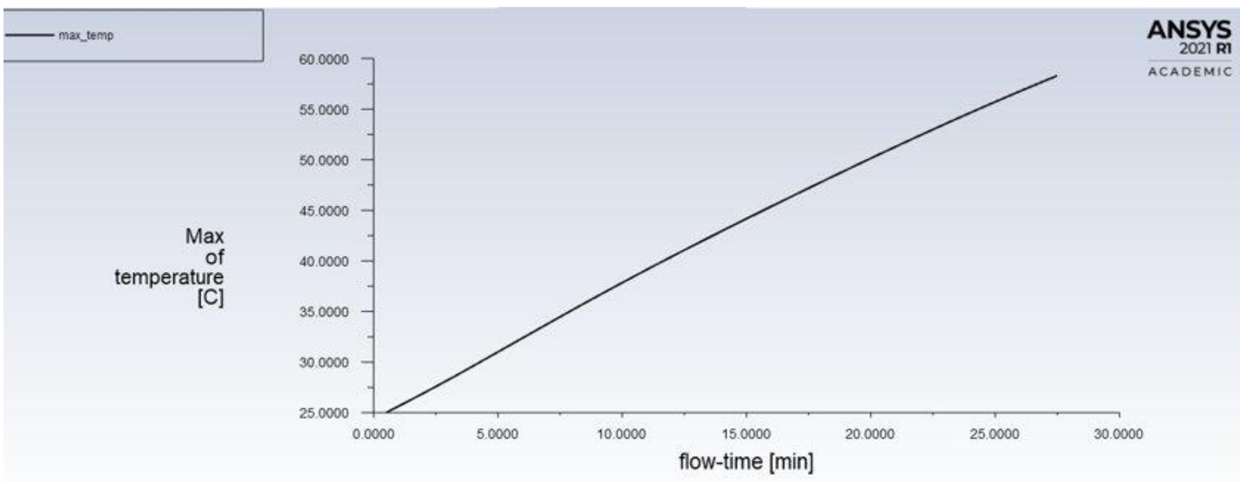


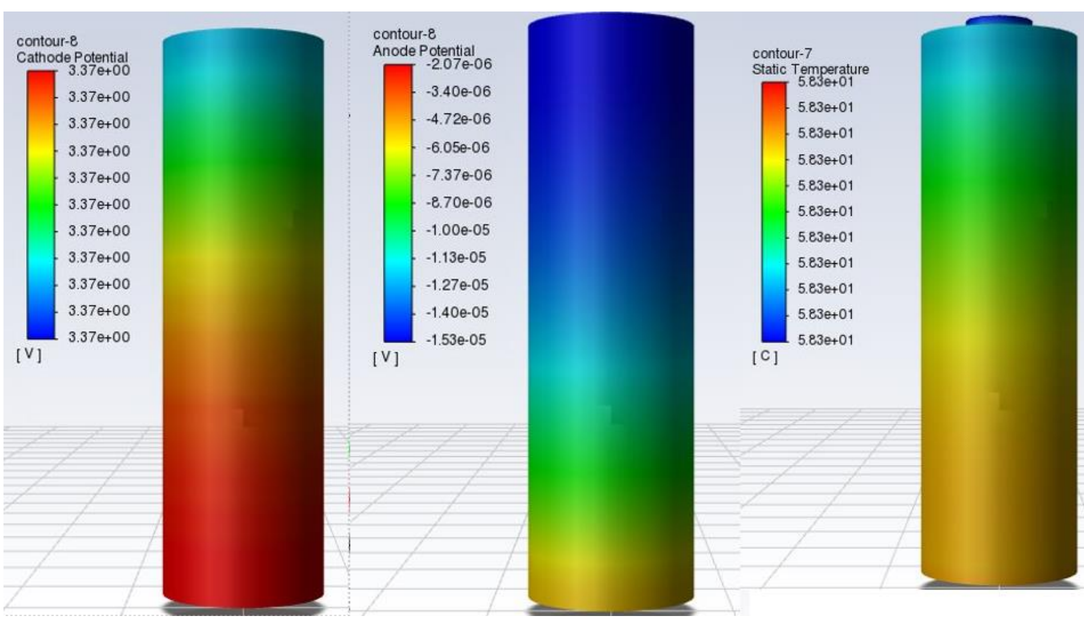


2C after fitting with 1C and 3C raw data:

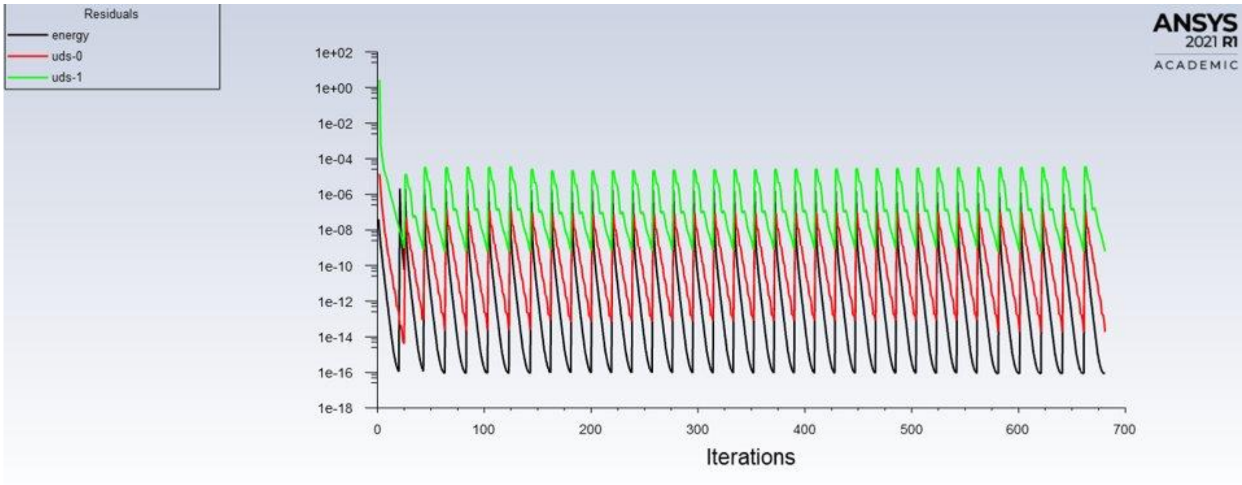


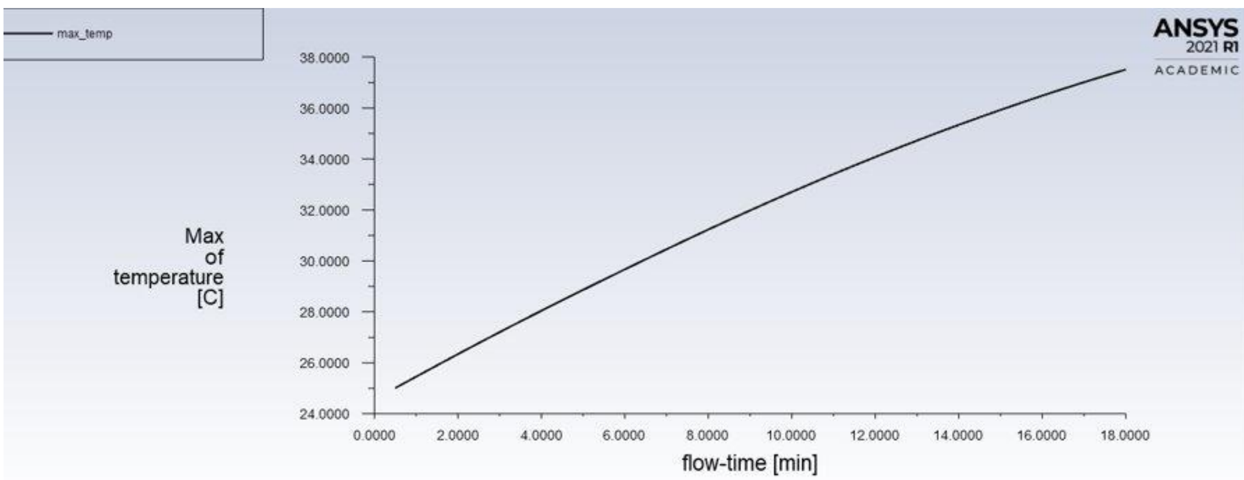

cellvoltage
ANSYS
2021 R1
ACADEMIC
Area-Weighted Average of cell-potential [V]
3.9000
3.8000
3.7000
3.6000
3.5000
3.4000
3.3000
0.0000
5.0000
10.0000
15.0000
20.0000
25.0000
30.0000
flow-time [min]

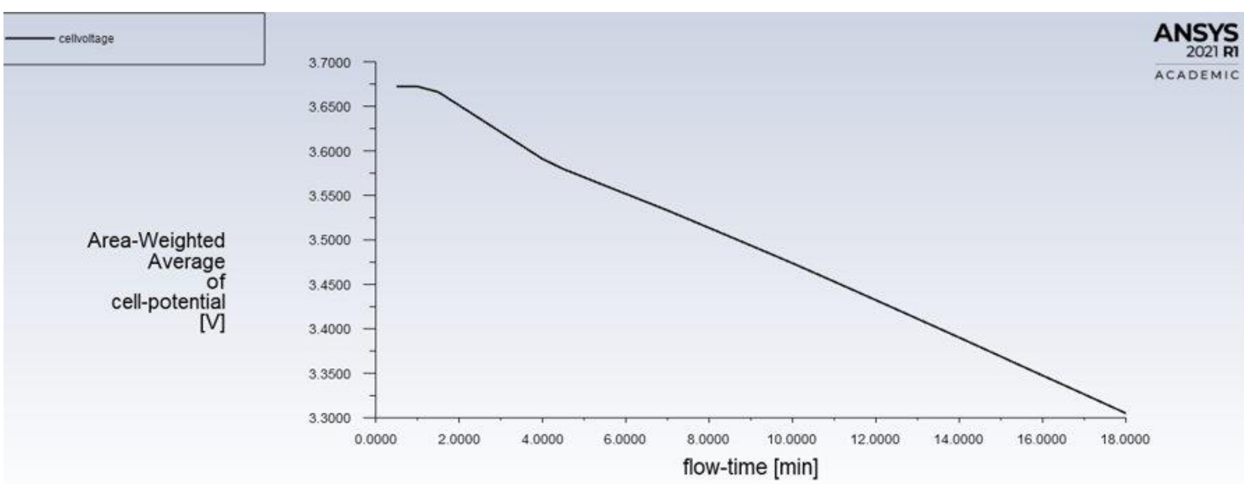

max_temp
ANSYS
2021 R1
ACADEMIC
Max of temperature [C]
60.0000
55.0000
50.0000
45.0000
40.0000
35.0000
30.0000
25.0000
0.0000
5.0000
10.0000
15.0000
20.0000
25.0000
30.0000
flow-time [min]

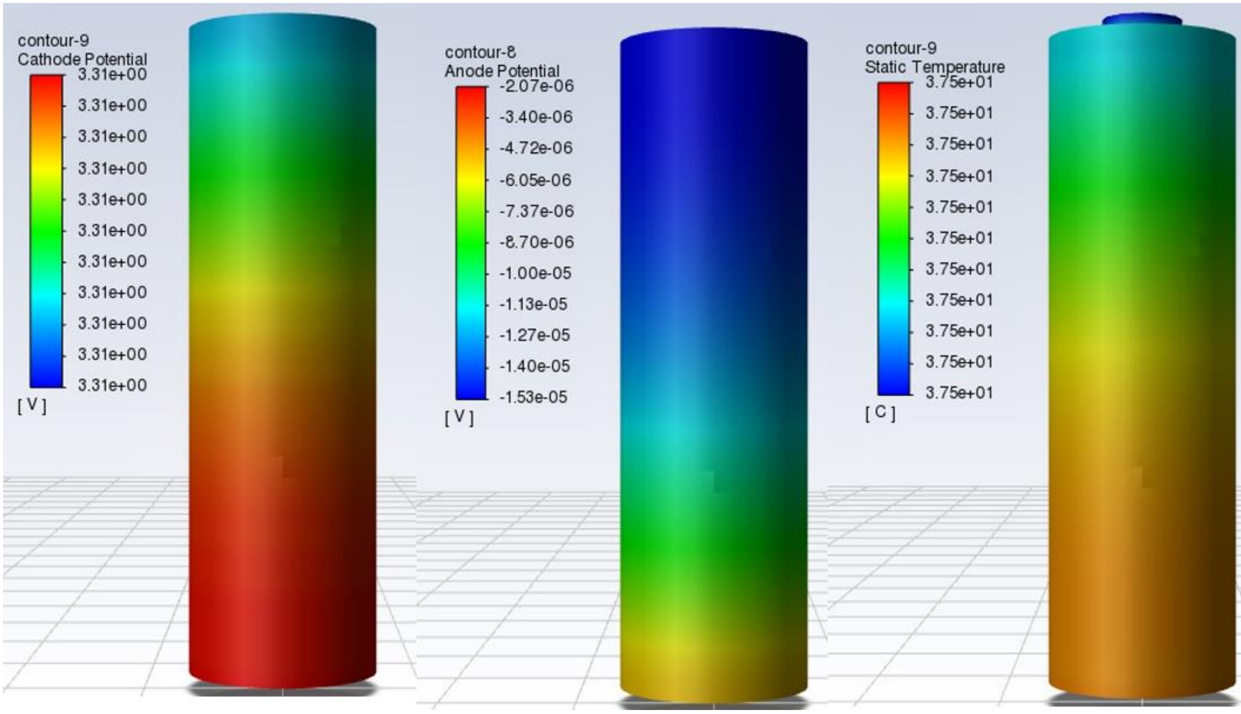

contour-8
Cathode Potential
3.37e+00
[V]
contour-8
Anode Potential
-2.07e-06
-3.40e-06
-4.72e-06
-6.05e-06
-7.37e-06
-8.70e-06
-1.00e-05
-1.13e-05
-1.27e-05
-1.40e-05
-1.53e-05
[V]
contour-7
Static Temperature
5.83e+01
[C]

3C after fitting with 2C and 5C:








contour-9
Cathode Potential
3.31e+00
3.31e+00
3.31e+00
3.31e+00
3.31e+00
3.31e+00
3.31e+00
3.31e+00
3.31e+00
3.31e+00
3.31e+00
[V]
contour-8
Anode Potential
-2.07e-06
-3.40e-06
-4.72e-06
-6.05e-06
-7.37e-06
-8.70e-06
-1.00e-05
-1.13e-05
-1.27e-05
-1.40e-05
-1.53e-05
[V]
contour-9
Static Temperature
3.75e+01
3.75e+01
3.75e+01
3.75e+01
3.75e+01
3.75e+01
3.75e+01
3.75e+01
3.75e+01
3.75e+01
3.75e+01
[C]