Imperial College London - Department of Mechanical Engineering

ME4-FCTT Future Clean Transport Technology 2022-23

Project 3: Modelling of lithium-ion batteries to understand limitations of performance

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Project administration

The schedule for Project 3 is shown in Table 1. The deadline is strict. Three tutorial sessions have been timetabled to answer queries about the project (attendance optional).

Table 1. Project 3 Schedule

Issued	20th Feb 2024
Deadline	Monday 18th Mar 2024, noon
Submission	• Online submission to Blackboard of report (.pdf) and code files. One set of files per group. Instructions of how to do this will be provided. • For work submitted up to 24 hours late, the mark will be capped at 40%. After this a zero mark will be given.
Tutorial 1	27th Feb, 4-5pm
Tutorial 2	5th Mar, 4-5pm
Tutorial 3	12th Mar, 4-5pm

- This project carries a maximum of one third of the 200 marks available for coursework. (The examination also carries 200 marks, giving a course total of 400 marks.)
- This project consists of four parts. Part 1 is worth 20%, Part 2 is worth 30%, Part 3 is worth 30%, Part 4 is worth 10%. The remaining marks will be attributed to the overall quality of the report. No further breakdown of the marking scheme will be provided.
- The report should be written as a technical report of your work, describing and explaining what you've done and how your model works. It should read on its own without the brief. You should **explain and justify steps taken to construct and parameterise** the model **in addition** to answering the explicitly stated questions.
- This project is marked on your understanding of battery fundamentals and how to model them. **You are not marked on how good your code is or the accuracy of your model fits**.
- After marking, a letter grade (A*–E) and feedback comments will be made available online. The number of marks awarded will not be announced.
- There will be an opportunity for peer review (using WebPA online software), whereby the contribution of an individual within each group is scored by the other group members, enabling up to a ±5% adjustment to the individual's project mark.
- There is no limit to the number of pages you can submit, and we are aware that different formatting styles will affect the length of the report. Please try to be concise. You should find that 30-35 pages (excluding any appendices) provide ample space to write a very good report.

Acronyms

State-of-charge (SOC)
Open circuit voltage (OCV)
Equivalent circuit network (ECN)
Constant Current-Constant Voltage (CC-CV)
Solid electrolyte interphase (SEI)

Data files provided

- Cell datasheets
- Battery-testing-data – against which you compare your model predictions
- Model-training-data – For parameterising your model
- SOC OCV – For parameterising your model
- Zip file RE_Data_for_Degradation – 4 files for parameterising your degradation model
- PyBaMM installation instructions
- PyBaMM running command file

Project brief

The purpose of this project is to reinforce your understanding of how lithium ion batteries behave, building upon the lectures on "Battery operating principles", "Thermal behaviour of batteries" and "Battery cell degradation". The scope of this project aligns with the behaviour of the majority of the automotive industry in their shift towards electrification and hybridisation of vehicles. This project will have you creating models to simulate the behaviour of a lithium ion battery cell. In reality, the behaviour of a lithium-ion battery is governed by highly complex electrochemical, physical and chemical processes. In this project you will be attempting to replicate this behaviour with simple electrical components and circuits. As your model becomes more complex, it will be able to capture more of the behaviour of the real cell.

Prepare a report (one per group) **including clear, detailed supporting calculations**, to answer the questions herein using the knowledge at your disposal, e.g., the materials in the modules presented so far, the recommended texts AND any other material you find. When using materials you have found, you must include an element of critical analysis of the credibility of the source.

We recommend that you attempt Part 1 and ideally also Part 2 parameterisation before the first tutorial.

Parallelisation of effort within your group (applies to all parts)

Some sections of the project can be developed in parallel to one another, once you understand how they relate to one another. The structure of the project is detailed in the flowcharts below, where the arrows highlight dependencies. **To aid your group in working in parallel, you have been provided with placeholder values to use in your model for Part 2 & 3 (these can be found at the start of Part 2 implementation). This will allow you to separate the work required for model construction and parametrisation.**

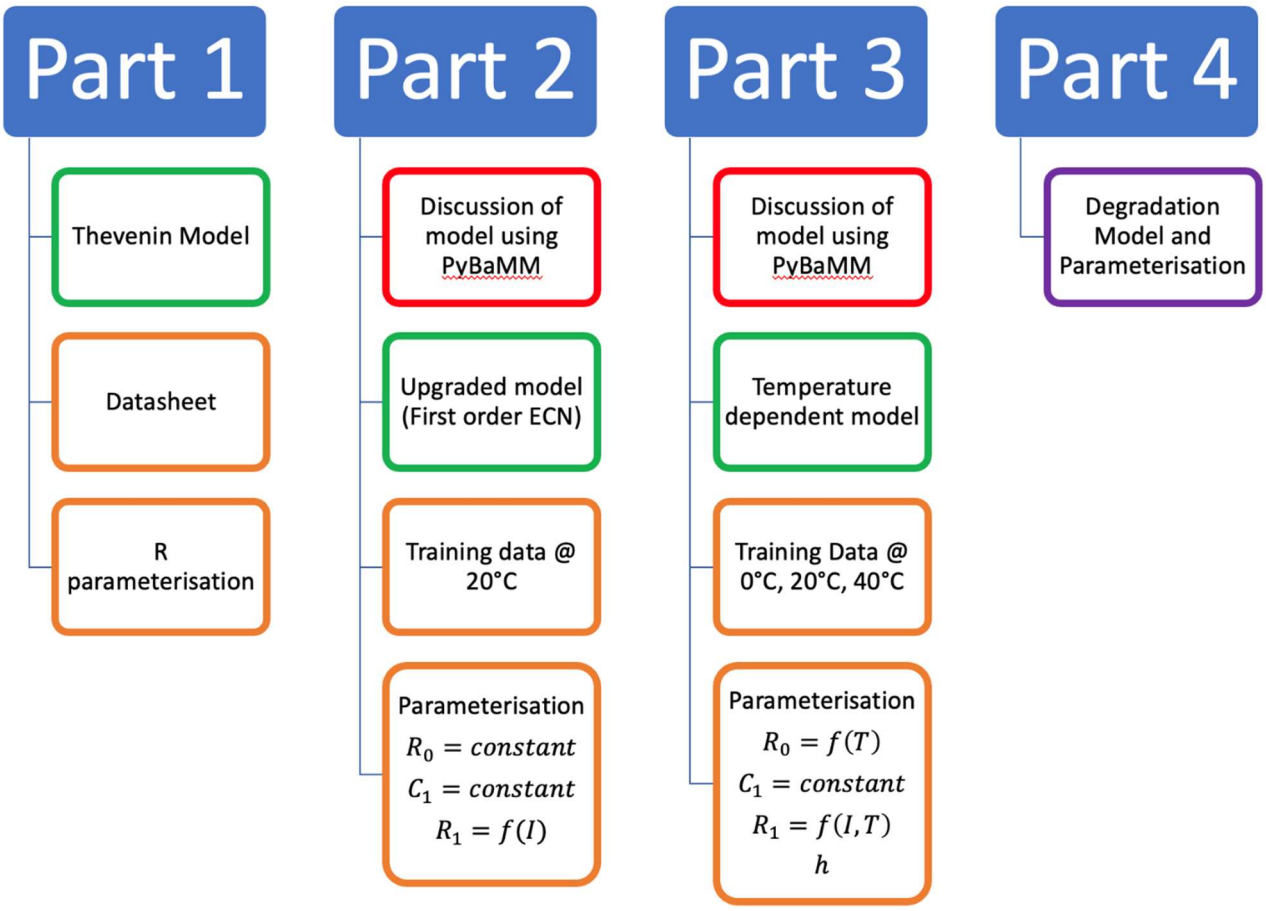

Figure 1: Flowchart of the content of this project - You will be building models (green frame) and parametrise them (orange frame). You are provided with code for the physics-based PyBaMM model to use in Part 2 and 3. The model and parametrisation you are creating in Part 4 is completely independent of the rest of the project.

Practical tips and advice

- 'Pair coding' is also strongly encouraged. This means that coders work in pairs and check each other's work. This is not the same as duplication of effort, as it has been found to dramatically reduce the number of coding errors, which usually pays off in the long run. Professional coding teams do this for a reason. There are particular ways of doing pair coding, including using repositories like GitHub, please look these up and share any best practice you learn with other teams.
- The use of **MATLAB OR Python** for calculations/model is advised. You are free to use other coding languages, but you would not receive any help in debugging if you were to do so. It is recommended to include snapshots of your code as an appendix to your report, but an electronic version of your models for must also be submitted.
- Using 3-D arrays or structs is advised.
- Using functions will help keep your code clean and make your code easier to debug.
- In the report, **comment on all presented results and fits**.
- Take care when presenting results in plots so that the features you discuss are clearly visible. The plots requested directly in this brief **are the minimum** expected, you may find other plots necessary to make the points you wish to discuss.

Part 1: Equivalent circuit network modelling of a lithium ion battery - Thévenin Model (20%)

In this first part you will model a lithium-ion battery cell with a simple equivalent circuit network (ECN) model. You will need to use the spec sheet of the lithium-ion battery provided. You are advised to read the lecture notes from Prof Gregory Plett[1] to gain an overview before attempting the questions. Please note that these resources contain more information and go into more detail than you need for this project. However, it is recommended you still read them completely for your understanding.

Model

In this part you should start by creating a Thévenin Model, which consists of a voltage source and single resistor. The input to the model is the current between the cell terminals as a function of time; the output of the model is the cell voltage as a function of time.

You are given:

- a spec sheet for the cell you will be modelling.
- a file called 'OCVdata', which contains the OCV as a function of SOC, as measured experimentally by a very slow discharge of the cell.
- a file called 'battery-testing-data', which contains a load profile in the form of current, voltage and temperature as functions of time. This data contains an initial CC-CV (constant current charge up to maximum voltage followed by constant voltage hold), and a long rest before the discharge of the cell begins. This data has been left in to aid your understanding of the 'history' of the cell, however **the questions will focus on the match between your model predictions and the drive cycle profile only**.

You will need to input the current profile as a function of time into your model, and compare the voltage predicted by the model against the experimentally measured voltage. The model can be made using a set of equations that use current as input to output a predicted voltage. You will need to use 'Coulomb counting' to track the State of Charge of the battery at all times during the load profile.

Parametrisation

In order to approximate the cell resistance 'R' for the Thévenin model, use the rate capability data given in the spec sheet (i.e. voltage curves for discharge at various current rates) and Ohm's law at 50% SOC.

Implementation

Using 'battery-testing-data' find the correct value of SOC to start your model at, such that your predicted voltage matches the real voltage just before the discharge profile begins.

Discussion

Using the model, do the following tasks and answer the following questions:

[1] http://mocha-java.uccs.edu/ECE5710/ECE5710-Notes02.pdf

a. Plot voltage against time, showing the voltage predicted by your model overlaid on the experimentally measured voltage (actual voltage).
b. Plot the error between the predicted and actual voltage as a function of time.
c. Describe the errors between the predicted and actual voltage. Carefully examine different parts of the drive cycle, identify where the most significant errors occur and provide physical reasons for them.

Part 2: Improvement of the model by introducing transient behaviour and current dependence (30%)

In this second part of the project, you will explore the effect of introducing transient behaviour and state dependent behaviour on the accuracy of the model.

Firstly, you will need to introduce a parallel combination of a resistor and capacitor into your model. An ECN model containing a resistor in series with a resistor and capacitor in parallel is known as a *first order ECN model* (i.e. a single RC pair in parallel). You will also need to re-parameterise your model, as the value for the series resistance cannot be directly taken as the value in Part 1.

You have been given a third file called 'model-training-data'[2] which contains a load profile in the form of current, voltage and temperature information as a function of time. This data represents the type of data that would be generated from experiments run with the aim to parametrise battery models. The experiments that have been conducted are:

The cell has been tested at 0^{o}C, 20^{o}C and 40^{o}C ambient temperature in a thermal chamber (i.e. oven with fan creating forced convection)

The cell has been discharged down to 8 SOC values, starting at 90% SOC in intervals of 10% SOC

At each SOC the cell has been subjected to 4 discharge and 4 charge pulses, of duration 10 seconds each, and of 4 different current magnitudes

Code Tips:

- Analyse all 8 SOCs automatically, i.e. via a script
- Think about how to automatically identify the beginning and end of each pulse

Discussion

Before adding complexity to your model, it is important to reflect on the phenomena that you are attempting to capture. We will use PyBaMM, a physics-based modelling tool as a virtual cell to "observe" the complex processes happening when you apply a discharge pulse.

PyBaMM uses a type of physics-based model called Pseudo-2D (P2D). This models the transport of lithium ions in the electrolyte (dimension 1) and of lithium atoms in the electrode particle (dimension 2 It also models the losses due to the kinetics limitations at the two electrode interfaces via the Butler Volmer equation, and takes in OCV data as a look up table from experiments (rather

[2] Note, that MATLAB can handle .csv files much easier than .xlsx

than the Nernst equation). The model also includes temperature dependence of the various voltage losses. The model does not account for any inhomogeneities within the cell other than those arising between the current collectors due to transport limitations.) This is similar to the analogy you will have seen in your lectures:

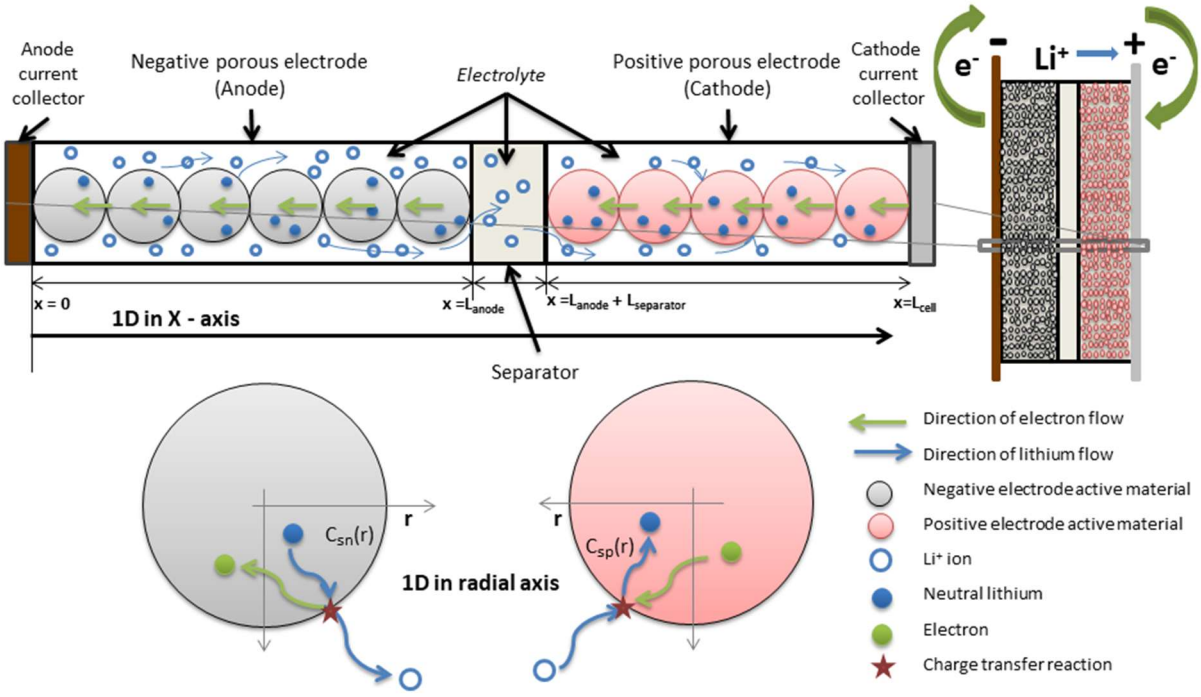

Figure 2: diagram of the structure of the Pseudo-2D model used by PyBaMM
https://www.ise.fraunhofer.de/en/simulations/electrical-and-electrochemical-modeling.html

Complex partial differential equations are used to model the movement of lithium inside the cell, which increases the computational cost of these models. The large number of parameters makes them challenging to parameterise.

Open the notebook titled FCTT_Project_3_PyBaMM.ipynb. Run each cell and answer the following questions. Once you run it, Figure 1 shows the developing overpotentials (voltage drops) that the cell experiences. Figure 2 shows the gradients inside the cell (between current collectors).

a. Describe the contributions to the voltage drop inside the cell when the current is applied. How do these relate to the circuit elements in your model? (Hint: identify the contributions that are instantaneous and those that are transient)
b. What are the largest contributions to the overpotential when the current is removed? From PyBaMM, plot the gradients inside the cell at the very end of the current pulse, and after the current has been removed and comment on the features that you observe.
c. Make a conclusion from your analysis: what is your Part 1 circuit model missing?

Parametrisation

To begin to parameterise your circuit model, complete the following steps.

a. For the data at 20°C, identify the data corresponding to each individual pulse and fit these to your first order ECN model. (Hint: a first order ECN model uses one series resistor and one RC pair; therefore, it should be modelled using one exponent.)
b. You should generate a table which has a value for R_0, R_1 and C_1 for each SOC and for each discharging and charging currents used in the experimental parametrisation data.
c. You should be able to see that R_0 does not depend on SOC and current magnitude in a meaningful manner – this is also what is expected from its physical interpretation. Thus, you may remove these dependencies. Take the average value for R_0 at all currents and SOCs and re-calculate values for R_1 and C_1.
d. What physical mechanisms does R_0 represent and what are you assuming by keeping it constant?
e. Plot the value of R_0 as a function of current at 60% SOC and comment on how accurate this assumption is.
f. Now take the average value for C_1 at all currents and SOCs, what are you assuming by keeping C_1 constant?
g. What physical mechanisms does the R-C pair represent? Relate them to the features that you observed in the PyBaMM model.
h. Plot the value of C_1 as a function of current at 60% SOC and comment on how accurate this assumption is.

You should now have values for R_0, C_1 that are constant, but values for R_1 that change with both current and SOC.

i. Plot the value of R_1 for 20°C and 60% SOC against current and describe the shape.

The mathematical function that best represents the physics between R_1 and current is a Gaussian function.

Fit R_1 for 20°C and 60% SOC to a first order Gaussian function as a function of current, and comment on the fit.

Equation 1 $$R_1 = R_1^{0A}.exp(-\frac{(I-b)^2}{c})$$

Where $R_1{}^{0A}$ is the resistance at open circuit, i.e. 0 A, and b and c do not have any physical meaning.

j. Attempt to improve your fit for R1 by adjusting the fitted equation (this can be done by changing the order or applying an offset).

(Note – you may find that the pulses do not go to small enough currents to enable you to obtain a Gaussian. You need to use the longer discharge periods, at low current to extract approximate R_1 values for smaller currents in discharge.)

Implementation

To enable you to work in parallel within your team, or to proceed with later parts of the project while still working on your parametrisation, you are provided below with a placeholder parameter set. If you do decide to build and test your model with these, remember to replace them with your parametrised values and equations, once you have them:

R0 = 40 mΩ

R1 = 5 mΩ

C1 = 5 kF

After following the parameterisation instructions above, you will have constant values for C_1 and R_0, and R_1 as a function of current.

Your model should accept current as a function of time as an input. Run the model and compare the voltage predicted by the model against the actual measured voltage.

Using 'battery-testing-data' find the correct value of SOC to start your model at, such that your predicted voltage matches the real voltage just before the discharge profile begins.

Discussion

Using the model, do the following and answer the following questions:

a. Plot voltage against time, showing your model voltage prediction overlaid on the actual voltage.
b. Plot the error between the predicted and actual voltage as a function of time.
c. Describe the errors between the predicted and actual voltage. Carefully examine different parts of the drive cycle, identify where the most significant errors occur and provide physical reasons for them. In your analysis, be sure to interpret your parameterisation: what are the effects of the assumptions you have made? Are your R and C values realistic?
d. Have the model predictions improved compared to those of the model in Part 1? Discuss the possible reasons for the difference in the predicting power of the two models, with reference to your answers from Part 1.
e. Discuss the remaining errors and make some suggestions how the model could be further improved to decrease them.

Part 3: Introducing a thermal model and thermal coupling (30%)

In this third part of the project, you will explore the effect of introducing a thermal model and thermal coupling on the usefulness of the model.

In Part 2, you parameterised your model at 20°C, but you have two additional datasets at 0°C and 40°C that are as yet unused. You will now use them to add temperature dependence to your model. In the real world, a cell generates heat when it is being used, and this heat affects the temperature of the cell, and thus its behaviour, i.e. voltage response. Therefore, your model must also be improved to predict this effect.

Discussion

Re-run your PyBaMM model, but increase the temperature to 333K:

a. Compare the model results between the two temperatures. Describe and explain the changes.

Parametrisation of R_0

Follow these steps to generate a relationship between R_0 and temperature:

a. Repeat steps a-b from "Parametrisation" in Part 2 for the data given at 0°C and 40°C
b. Use the value of C_1 at 20°C as a constant and re-calculate values for R_1.
c. Plot the value of R_0 (averaged over current) as a function of temperature at 60% SOC and describe its shape.
d. Fit the R_0 from (c) above in this section ("Parametrisation of R_0") to the Arrhenius equation as a function of temperature.

Equation 2: The Arrhenius equation $$R_0 = R_0^{T_0} \exp\left[-\frac{E}{R}\left(\frac{1}{T}-\frac{1}{T_0}\right)\right]$$

Where $R_0^{T_0}$ is the resistance at T_0, and T_0 here corresponds to 20°C, T is the temperature, R the gas constant, and E a fitting parameter.

e. How much does R_0 vary with temperature?
f. Explain the physical reasons behind why R_0 varies in this way with temperature.

Parametrisation of R_1

You will have generated values for R_1 across currents, temperatures and SOCs in the parts above.

a. Plot the value for R_1 at 0°C and -2.5A as a function of SOC
b. Comment on R_1 dependency on SOC
c. For simplicity, from here on, you will ignore the R_1 dependence on SOC. To continue parametrising your model, complete the following steps:
d. Plot the value of R_1 at 60% SOC and -2.5A as a function of temperature.
e. For the data plotted in c., fit R_1 to the Arrhenius equation to obtain R_1 as a function of temperature.

Equation 3 $$R_1 = R_1^{T_0} \exp\left[-\frac{E}{R}\left(\frac{1}{T}-\frac{1}{T_0}\right)\right], T_0 \text{ corresponds to } 20^oC$$

Plot the value of R_1 at -2.5A as a function of temperature, at 30% SOC and 90% separately.

f. On each of the two plots in e., overlay the Arrhenius equation using the values of $\mathrm{R}_1^{20^\circ\mathrm{C}}$ for that SOC, and the value of E as parametrised at 60%.
g. Discuss how accurate the Arrhenius equation with the same exponential factor is at predicting the behaviour of R_1 at different SOCs.
h. You can now combine the current dependence from part 2 with equation 3 to create a new function for R_1 that includes both the current and temperature dependence:

Equation 4 $$\mathrm{R}_1 = \mathrm{R}_1^{0\mathrm{A},20^\circ\mathrm{C}} \exp\left(-\frac{(\mathrm{I}-\mathrm{b})^2}{\mathrm{c}}\right) \exp\left(-\frac{\mathrm{E}}{\mathrm{R}}\left(\frac{1}{\mathrm{T}}-\frac{1}{\mathrm{T}_0}\right)\right)$$

where $\mathrm{R}_1^{0\mathrm{A},20^\circ\mathrm{C}}$ can be found as the result of fitting the data to Equation 4.

Note: Remember to add to this equation any adjustments you may have made to your Gaussian equation.

i. Plot the values for R1 at -20A as a function of temperature for the 3 SOCs. Comment on the possible reasons as to why R1 measurements at 0°C do not align on the exponential trend that may be fit through the values of R1(T) at the two higher temperatures. (Hint: Look at the raw training data and think about the meaning of this combination of current and temperature values.)

Implementation

You are going to ignore any thermal gradients within the cell and assume the cell can be modelled as a single lumped thermal mass. You are also going to ignore reversible heat, i.e. entropy. Your thermal model will operate under the following assumptions:

- Assume the cell can be modelled as a lumped thermal mass using the mass of the cell from the spec sheet and assume a specific heat capacity of 825 J kg^{-1} K^{-1}.
- Assume you can use Joule heating to model the heat generation in the cell.
- You will need to model heat transfer from the cell to the environment, assuming a generic heat transfer coefficient using $Q = hA(T_{\text{cell}} - T_{\text{env}})$. Adjust your value of *h* to achieve a good fit for the cell temperature.

Your model must be upgraded so that at each time step the heat *Q* generated from the ohmic and reaction heat and the heat transfer between the cell and the environment will update the cell temperature, taking into account the thermal mass of the cell. The temperature should then be carried forward to the next time step and affect the values of R_1 and R_2 and therefore the behaviour of the cell.

The only temperature inputs that should be provided is the starting cell temperature, and a constant ambient temperature.

Using 'battery-testing-data' find the correct value of SOC to start your model at, such that your predicted voltage matches the real voltage just before the discharge profile begins.

Parametrisation

If you were unable to generate fitting parameters in Part 2 you may use the placeholder parameter set, given at the start of Part 2 to parametrise your value of *h*.

Discussion

Using the model, answer the following questions:

a. Plot temperature against time and show your model prediction overlaid on the actual temperature.
b. Describe and justify your criteria for the parametrisation of *h*.
c. Comment on the value of *h* and compare to some typical values from literature, and consider what types of thermal management system could achieve this value of *h*.
d. Plot the error between the predicted and actual temperature as a function of time.
e. Plot voltage against time, showing your model voltage prediction overlaid on the actual voltage.
f. Plot the error between the predicted and actual voltage as a function of time.

g. Describe the errors between the predicted and actual voltage. Carefully examine different parts of the drive cycle, identifying where the most significant errors occur and providing physical reasons for them. In your analysis, be sure to interpret your parameterisation: What are the effects of the assumptions you have made? How have your methods impacted the magnitude of your R and C values?
h. Have the model predictions improved compared to those of the model in Part 2? Discuss the possible reasons for the difference in the predicting power of the two models, with reference to your answers from Part 2.
i. Discuss the remaining errors and make some suggestions how these could be reduced by further improvements to the model. Hint: the thermal chamber is controlled by bang-bang control.

Part 4: A simple degradation model (10%)

Degradation is a very complex process, influenced by many different external factors. However, under normal operating conditions a single degradation mechanism dominates, which is SEI layer growth. SEI layer growth has two main effects – lithium is consumed in the production of the SEI layer reducing capacity (known as capacity fade), and the resistance increases due to changes in the cells internal structure (known as power fade).

Temperature is the most dominant external influence that effects the rate of degradation. In addition, the voltage of the cell and the rate of charge/discharge can also have an effect on degradation. If extremes of voltage are avoided by using a limited capacity of the cell (SOC 90-10%), and the maximum rate of charge/discharge is relatively low (<2C), then these factors can be ignored. In this case degradation can be assumed to only be a function of the temperature and the energy throughput during cycling and a function of temperature and time during storage. Energy throughput is a more useful measure than number of cycles, as it takes into account that the full SOC window of the cell is not always used and that as the cell ages the energy throughput for a full cycle will decrease as the capacity degrades.

You have been provided with a very limited amount of information. However, the requirements for a typical automotive application are that the vehicle must be able to last for 150,000 miles over 10 years of operation.

The methodology in the paper by Cordoba-Arenas et. al. entitled “Capacity and power fade cycle-life model for plug-in hybrid electric vehicle lithium-ion battery cells containing blended spinel and layered-oxide positive electrodes” will be used to extrapolate data for cycle life and at different temperatures**. Read this paper and use it to find suitable values for the activation energy terms in the equations below.**

Cycle ageing model

It has been shown experimentally that the capacity fade can be described using a power law with energy throughput (Ah), and is related to temperature via an Arrhenius relationship. This means that the capacity loss ($S_{loss\ cycle}$), can be described using the equation below:

Equation 5 $$S_{loss\,cycle} = a_c \times exp\left(-\frac{E_{AC}}{RT}\right) \times Ah^{z_a}$$

Where a_c is fitting constant, E_{AC} is activation energy , R is the universal gas constant, T is temperature, Ah is energy throughput, and z_a is a power exponent.

Experimentally, it has been shown that resistance increase is linear with cycling, and therefore this can be described using a very similar equation to capacity fade, however without the power exponent and with a different activation energy E_{AR}:

Equation 6 $$R_{inc\ cycling} = a_R \times exp\left(-\frac{E_{AR}}{RT}\right) \times Ah$$

The above empirical relationships can be parameterised using the data provided in the Zip file RE_Data_for_Degradation at a single temperature. The data provided was based upon a 1C/1C charge/discharge at 45°C for 100% DoD, which is typical of that provided by cell manufacturers. The result can be extrapolated using the Arrhenius relationship to a wide range of temperatures.

Calendar ageing model

The method used to extrapolate calendar ageing was similar to that used for cycle ageing by assuming the degradation is also primarily driven by SEI layer growth, but this time replacing energy throughput with time. The equations used can be seen below:

Equation 7 $$\mathrm{S_{loss\ calendar}} = \mathrm{b_c} \times \exp\left(-\frac{\mathrm{E_{AC}}}{\mathrm{RT}}\right) \times \mathrm{time}^{\mathrm{z_b}}$$

Equation 8 $$R_{inc\ calendar} = b_R \times exp\left(-\frac{E_{AR}}{RT}\right) \times time$$

Where b_c, b_R, z_b are fitting constants, E_{AC} is activation energy (capacity), E_{AR} is activation energy (resistance), R is the universal gas constant, T is temperature and time is which cell is storage at a particular temperature.

The above empirical relationships can be parameterised using the data provided in the Zip file RE_Data_for_Degradation at a single temperature.

Implementation

Complete the following:

a. Plot capacity loss against energy throughput assuming that the cell is being cycled continuously for 5,000 hours at 1C/1C charge/discharge from 10°C to 60°C at 10°C increments.
b. Plot resistance increase against energy throughput assuming that the cell is being cycled continuously for 5,000 hours at 1C/1C charge/discharge from 10°C to 60°C at 10°C increments.
c. Plot capacity loss against storage time assuming that the cell is being stored for 10 years at 10°C to 60°C at 10°C increments.
d. Plot resistance increase against storage time assuming that the cell is being stored for 10 years at 10°C to 60°C at 10°C increments.

Discussion

a. Comment on the suitability of the data you have used to parameterise your model.

b. Consider how long an electric vehicle would last in a range of major cities around the world, assuming the battery pack was being stored at ambient temperature 95% of the time (i.e. sitting on the driveway). Assume that 30% capacity fade or 100% resistance increase corresponds to end of life.
c. Which regions of the world would you not sell your vehicles if you were offering an 8 year warranty?
d. How confident are you in your model's predictions?