Imperial College London - Department of Mechanical Engineering

ME4-MFCTT Future Clean Transport Technology 2018-19

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

Project administration

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

Table 1. Project 3 Schedule

Issued	During the lecture on Tuesday 19th February 2019
Deadline	Monday 11th March at noon on Blackboard
Submission	• Online submission to Blackboard of report (.pdf) and MATLAB 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	Thursday 28th February 3-4pm in CAGB 640
Tutorial 2	Thursday 7th March 3-4pm in SKEM 060

- 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 20%, Part 4 is worth 10% and Part 5 is worth 15%. The remaining 5% will be attributed to the overall quality of the report. No further breakdown of the marking scheme will be provided.
- After marking, a letter grade (A*–E) and feedback comments will be made available online. We cannot divulge the actual number of marks awarded.
- 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.
- Depending on your code, **Part 4 can take a significant time to run** (a couple of hours per temperature), ensure you leave sufficient time for debugging and to obtain results.

Acronyms

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

Data files provided

- Cell datasheets
- Battery-testing-data – For comparing your model predictions to
- 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

Project brief

This project is based around modelling a lithium ion battery. Its purpose is to reinforce your understanding of how lithium ion batteries behave, building upon the lectures on electrochemistry and lithium ion batteries. 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.

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, and the recommended texts, AND, any other material you find. When using material you have found, you must include an element of critical analysis of the credibility of the source.

The use of MATLAB for the calculations/model is required. It is recommended to include snapshots of your code as an appendix to your report, but an electronic version of your models for the 4 parts must also be submitted.

We recommend that you attempt at least Part 1 and perhaps also Part 2a & b before the first tutorial.

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 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 give yourself 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. In this part you should start by creating a Thévenin Model which consists of a voltage source and single resistor. You will need to create a forward facing model, which accepts current as a function of time as an input, and provides voltage as a function of time as an output. You are given a spec sheet for the cell you will be modelling, and any other values will be provided as you need them throughout the project. You have been given a file called 'OCV-data' which contains the OCV as a function of SOC.

You have also been given a file called 'battery-testing-data' which contains a load profile in the form of both current, voltage and temperature as a function of time. This data contains an initial CC-CV charge up to full and long rest before the load profile begins, this has been left in to aid your understanding, however the questions will focus on the match to the load profile.

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 actual voltage. The model can be made using a set of equations that use current to output a predicted voltage.

In order to evaluate the resistance 'R' for the Thévenin model use the rate capability data given in the spec sheet and Ohms law at 50% SOC.

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

Questions

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

1. Starting your model at 85% SOC and using 'battery-testing-data' plot voltage against time, showing your model prediction overlaid on the actual voltage.
2. Plot the error between the predicted and actual voltage as a function of time.
3. Describe the errors between the predicted and actual voltage.
   3.1. What is your maximum error and when?
   3.2. What happens when the current changes by a large amount quickly?
   3.3. Do the errors get smaller or larger as time increases?
4. Describe in general terms some possible physical reasons for these errors.

Notes

- Check that the Initial states match the data
- Don't forget the Coulomb counting in the voltage source, and how this defines the cell capacity

---

Part 2: Improvement of the model introducing transient behaviour, current and temperature 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 an RC pair into your model. An ECN model with a resistor in series with a resistor and capacitor in parallel, is known as a first order ECN model. You will also need to re-parameterise your model, as the original value for resistance is now incorrect. You have been given a third file called 'model-training-data'[2] which contains a load profile in the form of both current, voltage and temperature as a function of time. This data represents the type of data that would be generated from experiments designed to generate data for parameterisation of a model. The experiments that have been conducted are as follows:

a) The cell has been tested at 0°C, 20°C and 40°C
b) The cell has been discharged to 8 SOCs, starting at 90% with intervals of 10%
c) At each SOC the cell has been subject to 4 discharge and 4 charge pulses for 10 seconds at 4 different currents

MATLAB Tips

• Analyse all 8 SOCs in one loop • Think about how to automatically identify the beginning and end of pulses • Using 3-D arrays or structs is advised • Using functions will help keep your code clean and easier to debug

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

Part 2a transient behaviour and current dependence

To parameterise your model, complete the following steps. One of the problems in creating an ECN model, is that of extrapolation between the values measured at known points. There are multiple ways of approaching this, of which the three most common are. Putting the data in a lookup table and linearly interpolating between the known measurement points, fitting the data to a mathematical function and either generating a higher resolution lookup table, or using the mathematical function itself.

Questions

1. Comment on the advantages and disadvantages of the three approaches described above, and any other approaches you can think of.

In this project you will be making a number of assumptions, i.e. simplifications, in order to be able to fit your data to some simple mathematical functions and use them directly.

a) For the data at 20°C, identify the data corresponding to each individual pulse and fit these to your first order ECN model.
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
c) Take the average value for R_0 at all currents and SOCs and put this back into your model as a constant
d) Take the average value for C_1 at all currents and SOCs and put this back into your model as a constant
e) Refit the model to the data with the constant values of R_0 and C_1

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.

f) Plot the value of R_1 for 30°C and 60% SOC against current and describe the shape
g) Fit R_1 to a first order Gaussian function as a function of current

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.

Questions

1. What assumptions are you making by assuming that R_0 does not change and keeping it constant
2. Plot the value of R_0 as a function of current at 60% SOC and comment on how accurate this assumption is?
3. What assumption are you making by keeping C_1 constant?
4. Plot the value of C_1 as a function of current at 60% SOC and comment on how accurate this assumption is?

Part 2b temperature dependence of R_0

To parameterise your model, complete the following steps.

a) Repeat steps a-g for part 2a for the data given at 0°C and 40°C but using the value of C_1 at 20°C as a constant throughout.
b) Plot the value of R_0 as a function of temperature at 60% SOC and describe the shape
c) Fit R_0 to the Arrhenius equation as a function of temperature

Equation 2
$$R_0 = R_0^{20^oC}.exp^{\frac{-E}{R}\left(\frac{1}{T}-\frac{1}{T_0}\right)}$$

Where $R_0^{20^oC}$ is the resistance at 20°C, T is temperature, R is the gas constant, and E is the exponential factor.

Questions

1. How much does R_0 vary with temperature?
2. What physical process does R_0 represent?
3. Explain why R_0 varies in this way?

Part 2c temperature dependence of R_1

R_1 is more complicated, as it is a function of current, temperature and SOC.

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

From here on, we will ignore how it varies as a function of SOC.

To parameterise your model, complete the following steps.

a. Plot the value of R_1 at 60% SOC and -2.5A as a function of temperature
b. Fit R_1 to the Arrhenius equation to obtain R_1 as a function of temperature

Equation 3
$$R_1 = R_1^{20^oC}.exp^{\frac{-E}{R}\left(\frac{1}{T}-\frac{1}{T_0}\right)}$$

c. Plot the value of R_1 at 30% SOC and 90% separately as a function of temperature
d. On each graph overlay the Arrhenius equation using the values of $R_1^{20^oC}$ for that SOC but the value of E which was parameterised at 60%

Questions

1. Comment and discuss on how accurate the Arrhenius equation with the same exponential factor is at predicting the behaviour of R_1 at different SOCs

You can now combine these functions to create a new function for R_1 that includes both the current and temperature dependence.

Equation 4
$$R_1 = R_1^{0A,20^oC}.exp^{-\frac{(I-b)^2}{c}}.exp^{\frac{-E}{R}\left(\frac{1}{T}-\frac{1}{T_0}\right)}$$

2. Do you think temperature dependence of C_1 is needed?

Part 2d Implementation

You can now input the constant parameters for C_1 and implement R_0 as a function of temperature, and R_1 as a function of current and temperature in your model as variable parameters using the equations above.

You will also need to upgrade your model so that it accepts both current and temperature as a function of time as an input. You will then need to put both the current and temperature profile as a function of time into your model, and compare the voltage predicted by the model against the actual voltage.

Questions

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

1. Starting your model at 85% SOC and using 'battery-testing-data' plot voltage against time, showing your model prediction overlaid on the actual voltage.
2. Plot the error between the predicted and actual voltage as a function of time.
3. Describe the errors between the predicted and actual voltage.
   3.1. What is your maximum error and when?
   3.2. What happens when the current changes by a large amount quickly?
   3.3. Do the errors get smaller or larger as time increases?
4. Describe if the model has got better or worse compared to the model from Part 1. Discuss possible reasons why with reference to your answers from Part 1.
5. Discuss the remaining errors and make some suggestions how these could be improved.

Part 3: Introducing a thermal model and thermal coupling (20%)

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.

The model is already a function of temperature from part 2, but temperature is an input to the model and is therefore independent of what the model does. In the real world, a cell generates heat when it is being used, and this heat affects the operation of the cell. Therefore, your model must do the same.

For this part 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. To create your thermal model, complete the following steps.

a. 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}.
b. Assume you can use $P = I^2 R_0$ to model the ohmic heating

c. Assume you can use $P = I^2 R_1$ to model the reaction heat
d. You will need to model heat transfer from the cell to the environment, using $Q = hA(T_{cell} - T_{env})$ assuming a generic heat transfer coefficient h of 10 W m^{-2} K^{-1}

Your model must be upgraded so that at each time step Q generated from the ohmic and reaction heating and the heat transfer to or from the cell and the environment should 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.

You must also remove the temperature input into the model that you implemented in part 2, the only input that should be provided is the starting cell temperature, and the constant ambient temperature.

Questions

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

1. Starting your model at 85% SOC and using 'battery-testing-data' plot voltage against time, showing your model prediction overlaid on the actual voltage.
2. Plot temperature against time, and show your model prediction overlaid on the actual temperature.
3. Play around with your value of h until you get a good fit for the end of discharge
4. 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
5. For this final result plot, the error between the predicted and actual temperature as a function of time.
6. Discuss the remaining errors and make some suggestions how these could be improved.
   Hint: the thermal chamber is controlled by bang-bang control
7. Go back to Part 2c and plot the values for R_1 at -20A as a function of temperature for the 3 SOCs, comment on why at 0°C $R_1(T)$ does not appear to be exponential.

Part 4: Improvement of the model introducing a degradation mechanism (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.

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}), can be described using the equation below:

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

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 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:

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

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.

Implementation

$S_{loss\ cycle}$ does not need to be calculated at every time step, but can be calculated every 3,600 seconds (i.e. 1 hour) and then the parameter in the Coulomb counter in the voltage source which defines the cell capacity can be updated accordingly.

In the same way $R_{inc\ cycling}$ also does not need to be calculated at every time step, but can be calculated every 3,600 seconds (i.e. 1 hour) and then the parameter $R_1^{25^oC}$ should be increased accordingly.

Questions

1. Comment on the suitability of the data for this purpose.
2. Comment on the error that only updating the cell model from the degradation model every hour might introduce

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

$$S_{loss\ calendar} = b_c \times exp\left(-\frac{E_{ac}}{R_g T}\right) \times time^z$$

Equation 8

$$R_{inc\ calendar} = b_R \times exp\left(-\frac{E_{ac}}{R_g T}\right) \times time$$

Where b_c, b_R are fitting constants, E_{ac} is activation energy, R_g 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

The two degradation models must operate under different operating modes. When a load cycle is being applied to the model the cycle ageing model should be used to predict capacity fade and resistance increase. When current is not flowing through the model the calendar ageing model should be used to predict capacity fade and resistance increase. You must assume the effects are cumulative, i.e. the capacity fade and resistance increase carries forward, so that the calendar ageing model starts with the values that the cycle ageing model reached, and vice versa. Note, that this assumption is not necessarily true, and is the subject of ongoing research within the Department.

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

Questions

1. Comment on how long an electric vehicle battery pack would last assuming different operating temperatures, assuming that 30% capacity fade or 100% resistance increase is end-of-life
2. 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)
3. Which regions of the world would you not sell your vehicles if you were offering an 8 year warranty?

<u>Part 5: Final test (15%)</u>

Assuming the data file 'battery-testing-data' is representative of driving an electric vehicle through a city for 1 hour, and that the useable capacity of the battery is restricted between 85% and 10% SOC. Therefore, run the following through your model for a range of ambient temperature conditions ranging from 10°C to 40°C at 10°C increments.

- Run the 'battery-testing-data' profile starting at 85% SOC
- Charge your model at 0.5C until the SOC reaches 85%
- Run your Calendar ageing model for 11 hours and update the cell model accordingly
- Repeat 7,300 times or until one of the following occurs
    - Battery temperature exceeds 60°C
    - Battery voltage drops below 2.5V
    - SOC drops below 10%

Complete the following:

a. Plot capacity loss against time in years for the four ambient temperature conditions simulated above
b. Plot resistance increase against time in years for the four ambient temperature conditions simulated above

Questions

1. Do any of the simulations reach 7,300 repeats before failing
2. For any of the simulations that fail to reach 7,300 repeats before failing explain why
3. What would be the consequence of this study for vehicle battery pack designer