Created in COMSOL Multiphysics 6.2

Aging Analysis of a Lumped Battery Model

Introduction

Aging in batteries occurs due to multiple complex degradation phenomena and side reactions that are occurring simultaneously at different places in the battery. This tutorial demonstrates the Lumped Battery interface for modeling capacity loss in a lithium-ion battery.

A set of lumped parameters are used to describe the capacity loss that occurs due to parasitic reactions in the battery. Using a lumped modeling approach, assuming no knowledge of the internal structure or design of the battery electrodes or choice of materials, any aging model will have to be empirical, not being able to distinguish among different degradation phenomena. Typically, capacity loss and aging may be affected by the battery voltage, capacity throughput, aging history and temperature.

The aging analysis presented in this tutorial includes calendar life and cycle life studies.

Model Definition

The cell model is created using the Lumped Battery interface. The interface requires inputs such as the battery capacity, initial state of charge (SOC), an open circuit voltage versus SOC curve, and consists of lumped parameters that represent the ohmic, activation, and concentration overpotential contributions. A detailed description on how to optimize the parameters of the lumped model against experimental data can be found in the Application Libraries example Parameter Estimation of a Time-Dependent Lumped Battery Model.

The capacity fade that occurs in the battery due to parasitic reactions is modeled using the Capacity Loss node. The loss kinetics is specified using the in-built expression available in this node. The expression calculates a loss current based on a calendar aging time constant that defines the rate of the parasitic reactions, and dimensionless aging factors dependent on voltage, current, aging history and temperature. Finally, the loss current is used to calculate the accumulated capacity loss corresponding to the parasitic reactions.

In this tutorial, representative values have been used for the voltage and capacity loss lumped parameters. As an alternative, these parameters could have been obtained by parameter estimation (using an optimization solver) against available experimental data for calendar life and cycle life aging.

The temperature is set to 298.15 K in both studies.

CALENDAR LIFE ANALYSIS

A calendar life analysis involves aging the battery at open circuit at constant SOC. The potentiostatic mode of operation is used to maintaining the battery at a particular SOC. Calendar life aging analysis requires that aging factors dependent on voltage and aging history are included. The aging factor dependent on voltage relates to change in the parasitic reaction rate for different values of the battery voltage or SOC, and would correspond either to a parasitic electrochemical reduction reaction occurring on the negative electrode, or a parasitic oxidation reaction occurring on the positive electrode. The rate of capacity fade may decrease as a result of products formed by the parasitic reactions, for example by the formation of a mass-transport limiting film on the electrode particles. A decelerating aging rate is defined using the aging factor dependent on aging history. The calendar life aging study sets up a parametric sweep over three different applied battery voltages corresponding to the particular states-of-charge (25%, 50% and 100% SOC). The battery is aged for a period of two years in the calendar life study.

CYCLE LIFE ANALYSIS

A cycle life analysis of the battery is performed in the second part of the tutorial, where the battery is aged using a constant 1 C charge-discharge cycling scheme.

The Charge-discharge cycling mode of operation of the Lumped Battery interface is used to set up the 1 C cycling scheme, which starts with a 1 C discharge until the cell reaches a minimum voltage of 3.2 V, followed by a 500 s rest period, a 1 C charge until the cell attains a maximum voltage of 4.15 V, and finally a 500 s rest period.

Figure 1 shows the cell potential and current corresponding to the 1 C charge-discharge cycling scheme. The corresponding cell state-of-charge variation is shown in Figure 2.

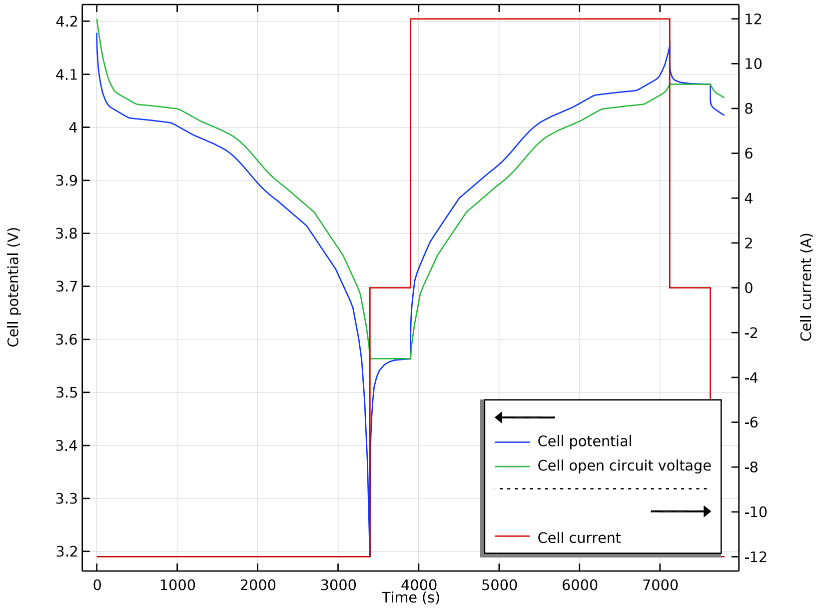

Figure 1: Cell potential and current corresponding to the 1 C charge-discharge cycling scheme.

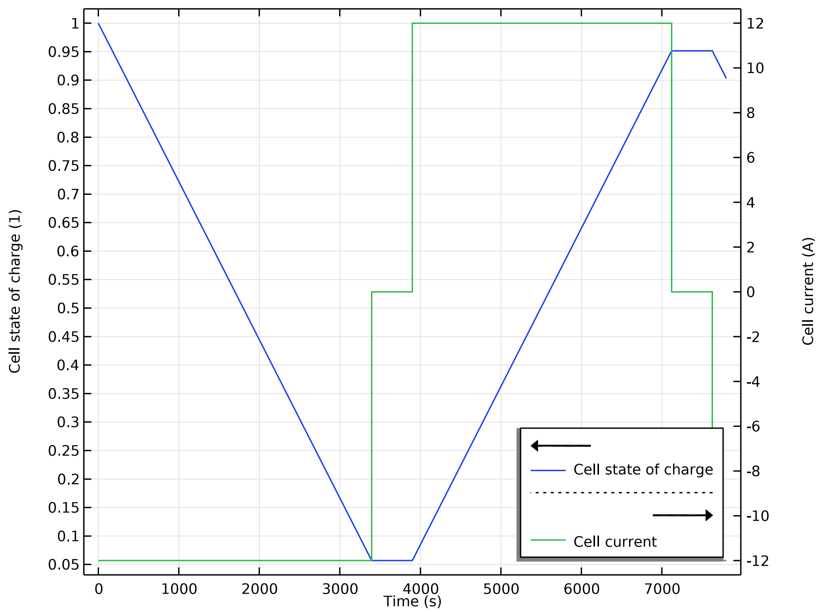

Figure 2: Cell state of charge and current corresponding to the 1 C charge-discharge cycling scheme.

In the cycle life aging analysis, the aging factor dependent on current is also included, in addition to the aging factors dependent on voltage and aging history. For many battery systems it is often observed that the lifetime is closely related to the amount of cycled equivalent full cycles (capacity throughput) and hence the aging factor dependent on current is used to define the additional capacity loss induced by cycling. The battery is aged for a period of 1 year in the cycle life study.

Results and Discussion

Figure 3 shows the cell state of health (SOH, relative cell capacity) variation with time, for the calendar life and cycle life studies.

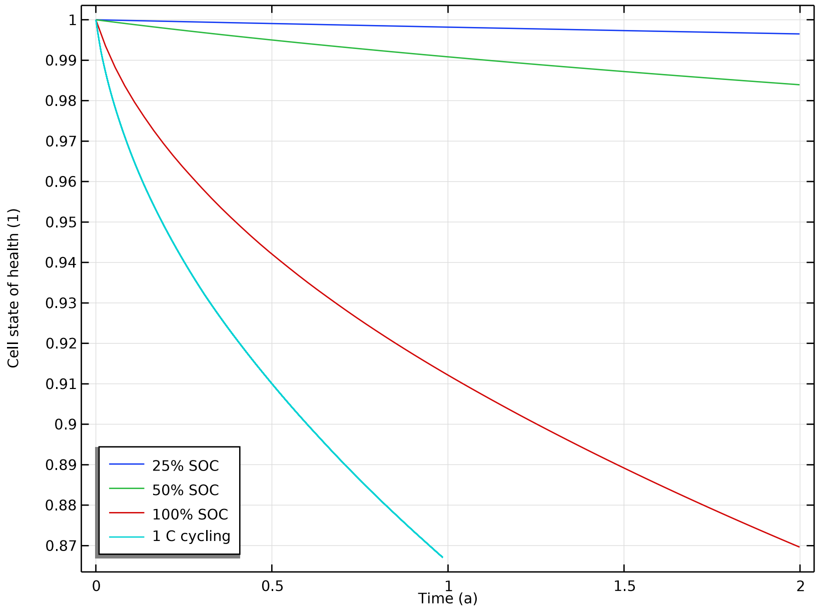

Figure 3: Cell state-of-health variation with time, for the calendar life and cycle life studies.

In many lithium-ion battery systems, it is seen that high SOC values (typically resulting in high battery voltage) accelerate capacity loss. The same is observed Figure 3, where the capacity loss is seen to be higher for calendar aging at higher SOC values. Additionally, the capacity loss is seen to be accelerated during the 1C cycle life aging.

The behavior seen in Figure 3 is similar to that typically observed for many battery systems. In this tutorial, representative values have been chosen for the lumped parameters describing capacity loss. Alternatively, these parameters can be obtained by parameter estimation (using an optimization solver) against available experimental data for calendar life and cycle life aging. Subsequently, the cell model using the optimized parameters can be used for capacity loss prediction of batteries aged using more complex cycling schemes.

Notes About the COMSOL Implementation

When computing the studies in the model file available in the Application Library, 'Study 1: Calendar Life' requires that the operation mode is set to Potentiostatic at the Lumped Battery interface level, and 'Study 2: Single Load Cycle' and 'Study 3: Cycle Life' require that the operation mode is set to Charge-discharge cycling at the Lumped Battery interface level.

Reference

1. H. Ekström and G. Lindbergh "A model for predicting capacity fade due to SEI formation in a commercial Graphite/$LiFePO_4$ cell," *J. Electrochemical Society*, vol. 162, pp. A1003–A1007, 2015.

Application Library path: `Battery_Design_Module/Batteries,_Lithium-Ion/lumped_li_battery_capacity_loss`

Modeling Instructions

From the **File** menu, choose **New**.

NEW

In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, click **0D**.

2 In the **Select Physics** tree, select **Electrochemistry>Batteries>Lumped Battery (lb)**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **General Studies>Time Dependent**.

6 Click **Done**.

GLOBAL DEFINITIONS

Parameters 1

Import the model parameters from a text file.

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

2 In the **Settings** window for **Parameters**, locate the **Parameters** section.

3 Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `lumped_li_battery_capacity_loss_parameters.txt`.

DEFINITIONS

Create an interpolation polynomial for the battery open circuit voltage from a text file. The function will be used later to specify the operating voltage, and the open circuit potential of the battery.

Interpolation 1 - E_OCP

1 In the **Home** toolbar, click f(X) **Functions** and choose **Local>Interpolation**.

2 In the **Settings** window for **Interpolation**, type `Interpolation 1 - E_OCP` in the **Label** text field.

3 Locate the **Definition** section. In the **Function name** text field, type `E_OCP`.

4 Click **Load from File**.

5 Browse to the model's Application Libraries folder and double-click the file `lumped_li_battery_capacity_loss_E_OCP_data.txt`.

LUMPED BATTERY (LB)

You will now start defining the battery model. A calendar life analysis of the battery is performed in the first part of the tutorial, where the battery is aged at open circuit at constant state of charge. **Potentiostatic** mode of operation is used for maintaining the battery at a particular state of charge.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Lumped Battery (lb)**.

2 In the **Settings** window for **Lumped Battery**, locate the **Operation Mode** section.

3 From the **Operation mode** list, choose **Potentiostatic**.

4 In the E_{app} text field, type `E_OCP(SOC_0)`.

5 Locate the **Battery Settings** section. In the $Q_{\mathrm{cell},0}$ text field, type `Q_cell0`.

6 In the $\mathrm{SOC}_{\mathrm{cell},0}$ text field, type `SOC_0`.

`Q_cell0` and `SOC_0` were defined in the parameter text file you imported before.

Cell Equilibrium Potential 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Lumped Battery (lb)** click **Cell Equilibrium Potential 1**.

2 In the **Settings** window for **Cell Equilibrium Potential**, locate the **Open Circuit Voltage** section.

3 From the **Open circuit voltage input** list, choose **From definitions**.

4 From the $E_{\mathrm{OCV,ref}}$ list, choose **Interpolation 1 - E_OCP (E_OCP)**.

Note that in this node you may also add data for the temperature derivative of open circuit voltage, that is used to calculate the temperature dependence of the open circuit voltage. Additionally, this data is used in the calculation of the reversible (entropic) contribution and heat of mixing contribution to the total heat source. However, this data is not needed in this model.

Voltage Losses 1

Specify the lumped parameter values for the voltage losses.

1 In the **Model Builder** window, click **Voltage Losses 1**.

2 In the **Settings** window for **Voltage Losses**, locate the **Model Input** section.

3 In the T text field, type `T`.

4 Locate the **Ohmic Overpotential** section. In the $\eta_{\mathrm{IR,1C}}$ text field, type `eta_IR_1C`.

5 Locate the **Activation Overpotential** section. In the J_0 text field, type `J0`.

6 Locate the **Concentration Overpotential** section. Select the **Include concentration overpotential** check box.

7 In the τ text field, type `tau`.

Capacity Loss 1

Add a **Capacity Loss** node to define the accumulated capacity loss in the battery corresponding to parasitic reactions. The loss kinetics is specified using the **Built in** option that calculates a loss current based on a **Calendar aging time constant** that defines the rate of the parasitic reactions, and dimensionless aging factors dependent on **Voltage**, **Current**, **Aging history** and **Temperature**, respectively.

1 In the **Physics** toolbar, click **Global** and choose **Capacity Loss**.

The calendar life aging study requires that aging factors dependent on **Voltage** and **Aging history** are included.

2 In the **Settings** window for **Capacity Loss**, locate the **Model Input** section.

3 In the T text field, type `T`.

4 Locate the **Capacity Loss** section. In the τ_{loss} text field, type `tau_loss`.

5 Select the **Voltage** check box.

6 In the E_{offset} text field, type `E_offset`.

7 In the α text field, type `alpha`.

8 Select the **Aging history** check box.

9 In the G text field, type `G`.

STUDY 1: CALENDAR LIFE

The first study performs a calendar life aging analysis of the battery, where the battery is aged at open circuit at constant state of charge. Set up a parametric sweep for different applied voltages corresponding to particular states-of-charge. The battery is aged for two years.

1 In the **Model Builder** window, click **Study 1**.

2 In the **Settings** window for **Study**, type `Study 1: Calendar Life` in the **Label** text field.

Parametric Sweep

1 In the **Study** toolbar, click **Parametric Sweep**.

2 In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.

3 Click **Add**.

4 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
SOC_0 (Initial state of charge)	`0.25 0.5 1`	

Step 1: Time Dependent

1 In the **Model Builder** window, click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

3 In the **Output times** text field, type `range(0,10[d],2[a])`.

4 In the **Model Builder** window, click **Study 1: Calendar Life**.

5 In the **Settings** window for **Study**, locate the **Study Settings** section.

6 Clear the **Generate default plots** check box.

7 In the **Study** toolbar, click **Compute**.

RESULTS

Proceed as follows to create a plot (Figure 3) for the cell state-of-health variation with time, at the different state of charge values.

Cell State-of-Health

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Cell State-of-Health` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1: Calendar Life/Parametric Solutions 1 (sol2)**.

Global 1

1 Right-click **Cell State-of-Health** and choose **Global**.

2 In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Lumped Battery>lb.SOH_cell - Cell state of health - 1**.

3 Locate the **x-Axis Data** section. From the **Unit** list, choose **a**.

4 Click to expand the **Legends** section. From the **Legends** list, choose **Evaluated**.

5 In the **Legend** text field, type `eval(SOC_0*100)% SOC`.

Cell State-of-Health

1 In the **Model Builder** window, click **Cell State-of-Health**.

2 In the **Settings** window for **1D Plot Group**, click to expand the **Title** section.

3 From the **Title type** list, choose **None**.

4 Locate the **Legend** section. From the **Position** list, choose **Lower left**.

5 In the **Cell State-of-Health** toolbar, click **Plot**.

LUMPED BATTERY (LB)

A cycle life aging analysis of the battery is performed in the second part of the tutorial, where the battery is aged using a constant 1C charge-discharge cycling scheme. **Charge-discharge cycling** mode of operation is used to set up the 1C cycling scheme (refer to Figure 1 and Figure 2). Note that `lb.I_1C` is the 1C current variable already available in the interface.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Lumped Battery (lb)**.

2 In the **Settings** window for **Lumped Battery**, locate the **Operation Mode** section.

3 From the **Operation mode** list, choose **Charge-discharge cycling**.

4 In the I_{dch} text field, type `-lb.I_1C`.

5 In the V_{min} text field, type `V_min`.

6 Select the **Include rest period** check box.

7 In the $t_{rest,dch}$ text field, type `t_rest`.

8 In the I_{ch} text field, type `lb.I_1C`.

9 In the V_{max} text field, type `V_max`.

10 Select the **Include rest period** check box.

11 In the $t_{rest,ch}$ text field, type `t_rest`.

Capacity Loss 1

The aging factor dependent on **Current** is also included for the cycle life study.

1 In the **Model Builder** window, under **Component 1 (comp1)>Lumped Battery (lb)** click **Capacity Loss 1**.

2 In the **Settings** window for **Capacity Loss**, locate the **Capacity Loss** section.

3 Select the **Current** check box.

4 In the H text field, type `H`.

ROOT

Add a study to first simulate a single cycle of the load that will be used in the cycle life aging analysis. Inspect the plots for the Cell Potential and Load (Figure 1) and Cell State of Charge (Figure 2) for a single cycle.

ADD STUDY

1 In the **Home** toolbar, click **Add Study** to open the **Add Study** window.

2 Go to the **Add Study** window.

3 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies> Time Dependent**.

4 Click **Add Study** in the window toolbar.

5 In the **Home** toolbar, click **Add Study** to close the **Add Study** window.

STUDY 2: SINGLE LOAD CYCLE

1 In the **Model Builder** window, click **Study 2**.

2 In the **Settings** window for **Study**, type `Study 2: Single Load Cycle` in the **Label** text field.

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 2: Single Load Cycle** click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

3 In the **Output times** text field, type `range(0,1,7800)`.

4 In the **Home** toolbar, click **Compute**.

RESULTS

Cell Potential and Load (Single Load Cycle)

1 In the **Settings** window for **1D Plot Group**, type `Cell Potential and Load (Single Load Cycle)` in the **Label** text field.

2 Click to expand the **Title** section. From the **Title type** list, choose **None**.

3 Locate the **Legend** section. From the **Position** list, choose **Lower right**.

Cell State of Charge (Single Load Cycle)

1 In the **Model Builder** window, under **Results** click **Cell State of Charge (lb)**.

2 In the **Settings** window for **1D Plot Group**, type `Cell State of Charge (Single Load Cycle)` in the **Label** text field.

3 Click to expand the **Title** section. From the **Title type** list, choose **None**.

4 Locate the **Legend** section. From the **Position** list, choose **Lower right**.

ROOT

Finally, add a third study to perform the cycle life aging analysis of the battery. The battery is aged for one year.

ADD STUDY

1 In the **Home** toolbar, click **Add Study** to open the **Add Study** window.

2 Go to the **Add Study** window.

3 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies> Time Dependent**.

4 Click **Add Study** in the window toolbar.

5 In the **Home** toolbar, click **Add Study** to close the **Add Study** window.

STUDY 3: CYCLE LIFE

1 In the **Model Builder** window, click **Study 3**.

2 In the **Settings** window for **Study**, type `Study 3: Cycle Life` in the **Label** text field.

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 3: Cycle Life** click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

3 In the **Output times** text field, type `range(0,10[d],1[a])`.

4 In the **Model Builder** window, click **Study 3: Cycle Life**.

5 In the **Settings** window for **Study**, locate the **Study Settings** section.

6 Clear the **Generate default plots** check box.

7 In the **Home** toolbar, click **Compute**.

RESULTS

Cell State-of-Health

Proceed as follows to include the cycle life data in the Cell State-of-Health plot (Figure 3).

Global 1

In the **Model Builder** window, right-click **Global 1** and choose **Duplicate**.

Global 2

1 In the **Model Builder** window, click **Global 2**.

2 In the **Settings** window for **Global**, locate the **Data** section.

3 From the **Dataset** list, choose **Study 3: Cycle Life/Solution 7 (sol7)**.

4 Click to expand the **Legends** section. From the **Legends** list, choose **Manual**.

5 In the table, enter the following settings:

Legends
`1 C cycling`

Cell State-of-Health

1 In the **Model Builder** window, click **Cell State-of-Health**.

2 In the **Cell State-of-Health** toolbar, click **Plot**.