Created in COMSOL Multiphysics 6.3

Parameter Estimation of a Time-Dependent Lumped Battery Model

Introduction

This tutorial uses a “black-box” approach to define a battery model based on a small set of lumped parameters, requiring no knowledge of the internal structure or design of the battery electrodes, or choice of materials. The inputs to the model are the battery capacity, the initial state-of-charge (SOC), and an open circuit voltage versus SOC curve, in combination with load cycle experimental data.

Parameter estimation of the lumped parameters is achieved using the Parameter Estimation study step.

Model Definition

The model could be seen as a lumped version of a single particle model, modeling the transport of intercalated lithium in one of the electrodes. This simplification can be motivated as long as the battery is mainly governed by the diffusion process in one of the electrodes only. The single particle modeling approach is exemplified in the Application Library example Single-Particle Modeling of Lithium-Ion Batteries.

This model uses the Lumped Battery interface and calculates the battery cell voltage E_{cell} (V) subject to an applied time-dependent cell current I_{cell} (A). The parameters used in the model are described in Table 1. Additionally, the model requires the battery open circuit voltage data, E_{OCV} (V), as function of state-of-charge.

TABLE 1: MODEL PARAMETERS.

PARAMETER	UNIT	DESCRIPTION
$Q_{\mathrm{cell,0}}$	A·h	Battery capacity
SOC_0	1	Initial state-of-charge
$\eta_{\mathrm{IR,1C}}$	V	Ohmic overpotential at 1C
J_0	1	Dimensionless charge exchange current
τ	s	Diffusion time constant

POTENTIAL LOSSES DUE TO OHMIC AND CHARGE TRANSFER PROCESSES

The lumped voltage loss associated with ohmic process in the electrolyte and electrodes is given as,

$$\eta_{\mathrm{IR}} = \eta_{\mathrm{IR,1C}}\frac{I_{\mathrm{cell}}}{I_{\mathrm{1C}}}$$

where $\eta_{IR,1C}$ (V) is the ohmic overpotential at 1C, I_{cell} is the applied current, and the 1C current, I_{1C} (A), is defined as,

$$I_{1C} = \frac{Q_{cell,0}}{3600\ \mathrm{s}}$$

where $Q_{cell,0}$ (C) is the battery cell capacity.

The dimensionless charge exchange current J_0 is used to define the lumped voltage loss associated with the charge transfer reactions (activation overpotential) on both the positive and negative electrode surfaces as

$$\eta_{act} = \frac{2RT}{F}\operatorname{asinh}\left(\frac{I_{cell}}{2J_0 I_{1C}}\right)$$

where R denotes the molar gas constant, T the temperature, and F Faraday's constant.

POTENTIAL LOSS DUE TO DIFFUSION PROCESSES

Concentration overpotential effects can be accounted for in the Lumped Battery interface either based on diffusion in an idealized particle or by using an RC pair (a linear resistor coupled in parallel with a capacitor). In this model, particle diffusion is considered. In this case, Fickian diffusion of a dimensionless SOC variable is solved for in a 1D pseudo extra dimension corresponding to the particle dimension of length 1 with X as the dimensionless spatial variable, using spherical symmetry (for spherical particles), according to

$$\tau\frac{\partial \mathrm{SOC}}{\partial t} = -\nabla\cdot(-\nabla\mathrm{SOC})$$

where τ (s) is the diffusion time constant. The interval represents an average particle of the electrode governing the battery, where $X = 0$ and $X = 1$ represent the center and surface of the particle, respectively.

The boundary conditions at the center and surface of the particle are as follows:

$$\nabla\mathrm{SOC} = 0\big|_{X=0}$$
$$\nabla\mathrm{SOC} = \frac{\tau I_{cell}}{N_{shape}Q_{cell,0}}\bigg|_{X=1}$$

where N_{shape} is 3 for spherical particles. The initial cell state-of-charge is specified by SOC_0. The surface state-of-charge, $\mathrm{SOC}_{surface}$, is defined at the surface of the particle

($X = 1$). The average state-of-charge, $\mathrm{SOC}_{\mathrm{average}}$, is defined by integrating over the volume of the particle, appropriately considering spherical coordinates, and is defined as

$$\mathrm{SOC}_{\mathrm{average}} = \frac{\int_0^1 \mathrm{SOC}\,4\Pi X^2 \mathrm{d}X}{\int_0^1 4\Pi X^2 \mathrm{d}X} = 3\int_0^1 \mathrm{SOC}\,X^2 \mathrm{d}X \qquad (1)$$

The lumped voltage loss associated with concentration overpotential is defined as,

$$\eta_{\mathrm{conc}} = E_{\mathrm{OCV}}(\mathrm{SOC}_{\mathrm{surface}}) - E_{\mathrm{OCV}}(\mathrm{SOC}_{\mathrm{average}})$$

CELL POTENTIAL AND PARAMETER ESTIMATION

Finally, the battery cell voltage E_{cell} is defined as

$$E_{\mathrm{cell}} = E_{\mathrm{OCV}}(\mathrm{SOC}_{\mathrm{average}}) + \eta_{\mathrm{IR}} + \eta_{\mathrm{act}} + \eta_{\mathrm{conc}}$$

Introducing the expression for η_{conc}, E_{cell} can also be defined as

$$E_{\mathrm{cell}} = E_{\mathrm{OCV}}(\mathrm{SOC}_{\mathrm{surface}}) + \eta_{\mathrm{IR}} + \eta_{\mathrm{act}}$$

The tutorial consists of three parts. In the first part, a lumped battery model (of capacity 12 Ah) is set up and run for a time-dependent battery current. In the second part, parameter estimation of the parameters $\eta_{\mathrm{IR,1C}}$, τ, and J_0, is performed using experimental data. This is done using a Parameter Estimation study step using a Levenberg–Marquardt optimization solver. In the third part, cell voltage prediction is performed using the optimized lumped parameter values that were obtained in the previous parameter estimation study, and compared with experimental data. The first two studies use a 300 s load cycle. The third prediction study uses a full load cycle with additional 300 s.

Results and Discussion

Figure 1 shows the modeled cell voltage using the fitted parameter values from Table 2 together with the experimental cell voltage and the corresponding open circuit voltage, for the 300 s load cycle.

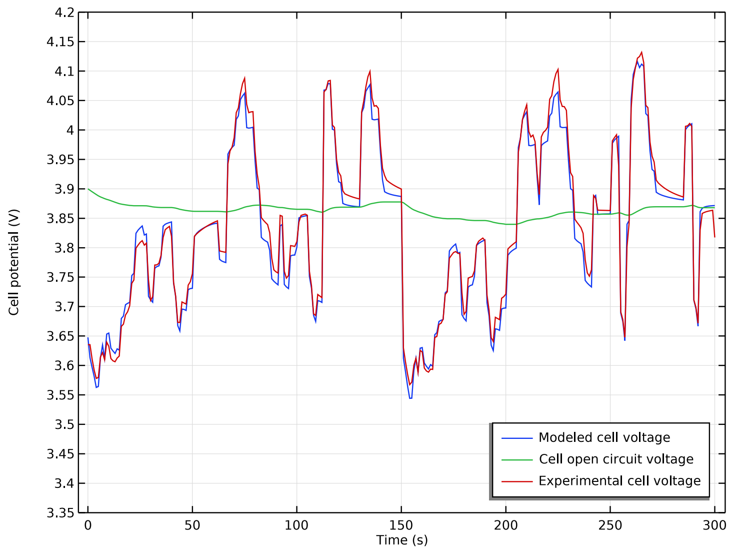


Figure 1: Modeled cell voltage using the fitted parameter values, experimental cell voltage, and corresponding open circuit voltage, for the 300 s load cycle.

TABLE 2: FITTED PARAMETER VALUES.

PARAMETER	VALUE	UNIT
$\eta_{IR,1C}$	4.5	mV
J_0	1.16	1
τ	1375	s

[Figure 2] shows the ohmic, activation, and concentration related voltage losses for the 300 s load cycle using the fitted parameter values.

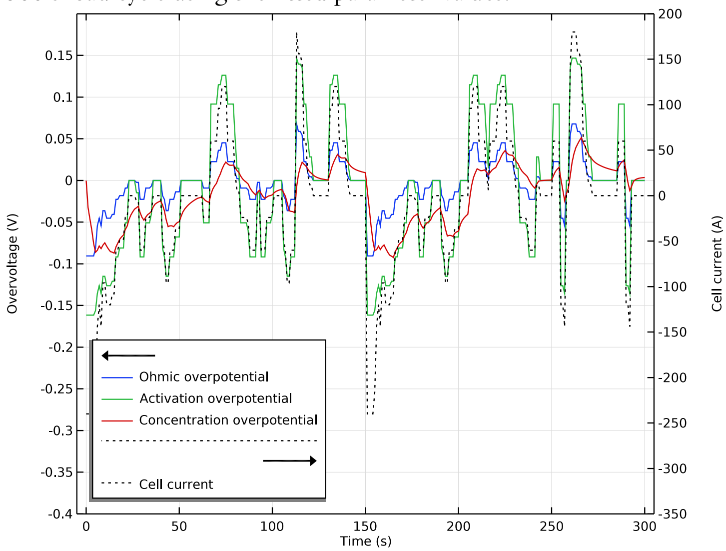


Figure 2: Ohmic, charge transfer and concentration voltage losses using the fitted parameter values, for the 300 s load cycle. Corresponding cell current load shown on second y-axis.

Figure 3 shows the predicted cell voltage using the optimized parameter values from Table 2 together with the experimental cell voltage and the corresponding open circuit voltage, for the full 600 s load cycle. (Note that the first half (300 s) of the predicted cell voltage is exactly similar to Figure 1, as expected).

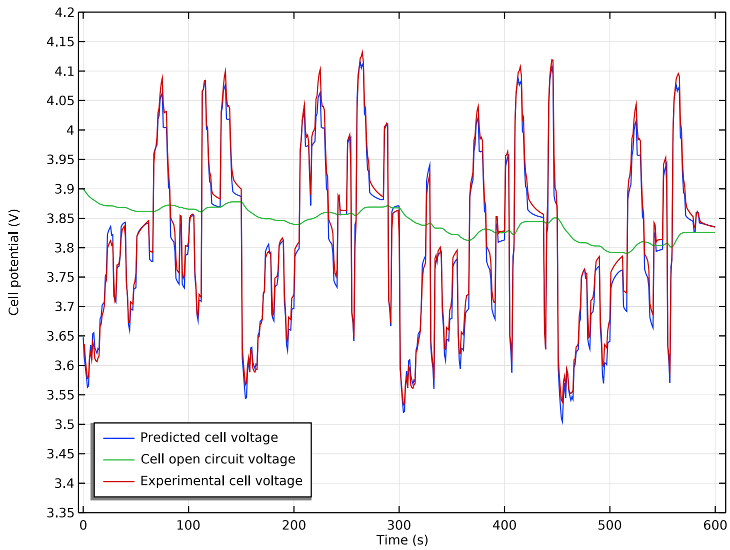


Figure 3: Predicted cell voltage using the optimized parameter values, experimental cell voltage, and corresponding open circuit voltage, for the full 600 s load cycle.

TABLE 3: STANDARD DEVIATION: CELL VOLTAGE.

STUDY	**STANDARD DEVIATION**
Load curve simulation	0.031
Parameter estimation	0.015
Full load curve prediction	0.014

The standard deviation values of the modeled cell voltage from the experimental values for all the three studies is shown in Table 3. The standard deviation value of first Load curve simulation study is high, as expected, considering that default values of the lumped parameters are used to simulate the cell voltage. The standard deviation value of the second Parameter estimation study and the third Full load curve prediction study are much lower and nearly the same. (Note that the standard deviation calculation of the prediction study uses only the latter half of the full load cycle). The nearly identical standard deviation values of the second and third study indicate that the quality of prediction will be only as good as the quality of parameter estimation and optimization.

Notes About the COMSOL Implementation

In the model, the inverse of J_0, `invJ0`, is used as fitting parameter. This is done in order to avoid division by 0 in the activation overpotential expression during the optimization process.

Reference

1. H. Ekström, B. Fridholm, and G. Lindbergh, "Comparison of lumped diffusion models for voltage prediction of a lithium-ion battery cell during dynamic loads," *J. Power Sources*, vol. 402, pp. 296–300, 2018.

Application Library path: `Battery_Design_Module/Lithium-Ion_Batteries, _Performance/lumped_li_battery_parameter_estimation`

Modeling Instructions

This tutorial consists of three parts. In the first part you will learn how to build a lumped battery model and run a simulation for a time-dependent battery current. In the second part you will perform parameter estimation using experimental data. In the third part, you will perform a prediction study using the optimized lumped parameter values that were obtained in the previous parameter estimation study, and compare with experimental data.

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_parameter_estimation_parameters.txt`.

DEFINITIONS

The battery current and the experimental cell voltage are time-dependent. Therefore you need to define these as variables. (The experimental cell voltage variable will only be used during postprocessing.)

Variables 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Definitions** and choose **Variables**.

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

3 Click **Load from File**.

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

   The expressions in the variable list are marked in orange, indicating unknown operators and functions. You will now proceed to add the missing interpolation function for the cell voltage and current versus time.

RESULTS

We will import the battery load and experimental cell voltage data as a table, and use this table both for defining time-dependent battery current and experimental voltage functions, as well as for the objective function used in the second part of the tutorial.

Load Cycle Data

1 In the **Model Builder** window, expand the **Results** node.

2 Right-click **Results** > **Tables** and choose **Table**.

3 In the **Settings** window for **Table**, type `Load Cycle Data` in the **Label** text field.

4 Locate the **Data** section. Click **Import**.

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

LOAD CYCLE DATA

1 Go to the **Load Cycle Data** window.

The data file contains three different columns: Time, Current and Voltage.

DEFINITIONS

Interpolation - E and I vs. t

1 In the **Definitions** toolbar, click **Interpolation**.

2 In the **Settings** window for **Interpolation**, type `Interpolation - E and I vs. t` in the **Label** text field.

3 Locate the **Definition** section. From the **Data source** list, choose **Result table**.

(Note that, instead of using the table, you could have imported the data file directly here too.)

4 Locate the **Data Column Settings** section. In the table, click to select the cell at row number 1 and column number 1.

5 In the **Unit** text field, type `s`.

6 In the table, click to select the cell at row number 2 and column number 1.

7 In the **Name** text field, type `E_cell_exp`.

8 In the table, enter the following settings:

Columns	Type	Settings
Current (A)	Function values	Function name=I_cell_exp

9 In the **Name** text field, type `I_cell_exp`.

LUMPED BATTERY (LB)

You will now start defining the battery model.

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 In the I_{app} text field, type `I_cell_exp`.

4 Locate the **Initial Capacity** section. In the $Q_{\mathrm{cell,0}}$ text field, type `Q_cell0`.

5 Locate the **Initial Cell Charge Distribution** section. In the $SOC_{cell,0}$ text field, type `SOC_0`.

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

(The **Battery volume** parameter is only used to calculate the heat source, in the unit W/ m^3, and is not needed in this model.)

Cell Equilibrium Potential 1

Load the open circuit voltage data at the reference temperature from a text file. Note that in this model the reference temperature is same as the simulation temperature.

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 Click **Clear Table**.

Note that it is important to clear the table before loading data from the text file.

4 Click **Load from File**.

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

6 In the T_{ref} text field, type `T`.

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

Keep the default values for the **Voltage Losses** parameters for now, but enable also the concentration overpotential.

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

2 In the **Settings** window for **Voltage Losses**, locate the **Concentration Overpotential** section.

3 Select the **Include concentration overpotential** checkbox.

STUDY 1 - LOAD CURVE SIMULATION

The battery model is now ready for solving.

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

2 In the **Settings** window for **Study**, type `Study 1 - Load Curve Simulation` in the **Label** text field.

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 1 - Load Curve Simulation** 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(0,1,300)`.

The above setting tells the solver to run a simulation for 300 s and store the solution every second.

4 From the **Tolerance** list, choose **User controlled**.

5 In the **Relative tolerance** text field, type `0.001`.

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

RESULTS

Cell Voltage

A number of plots were created by default. You will now modify the first plot to compare the modeled cell voltage with the experimental data.

1 In the **Settings** window for **1D Plot Group**, type `Cell Voltage` in the **Label** text field.

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

3 Locate the **Plot Settings** section. Clear the **Two y-axes** checkbox.

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

Global 1

1 In the **Model Builder** window, expand the **Cell Voltage** node, then click **Global 1**.

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

3 In the table, enter the following settings:

Expression	Unit	Description
lb.E_cell	V	Modeled cell voltage

Global 3

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

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)** > **Definitions** > **Variables** > **E_cell_exp - Experimental cell voltage - V**.

Cell Voltage

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

2 In the **Settings** window for **1D Plot Group**, locate the **Axis** section.

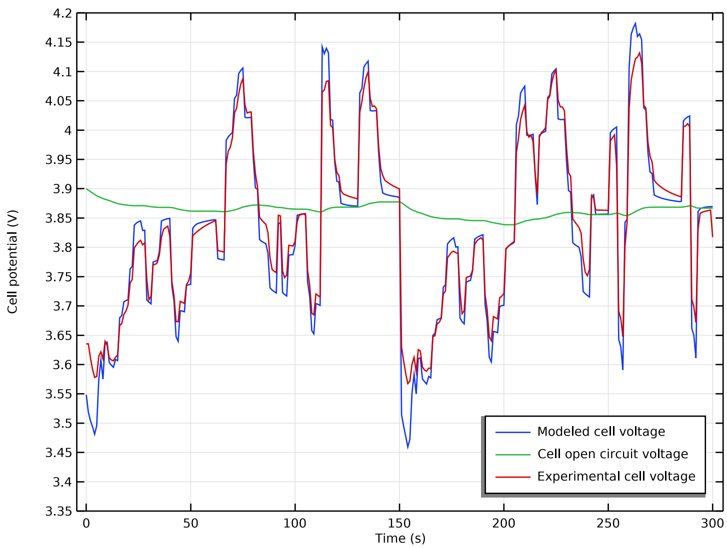
3 Select the **Manual axis limits** checkbox.

4 In the **x maximum** text field, type `305`.

5 In the **y minimum** text field, type `3.35`.

6 In the **y maximum** text field, type `4.2`.

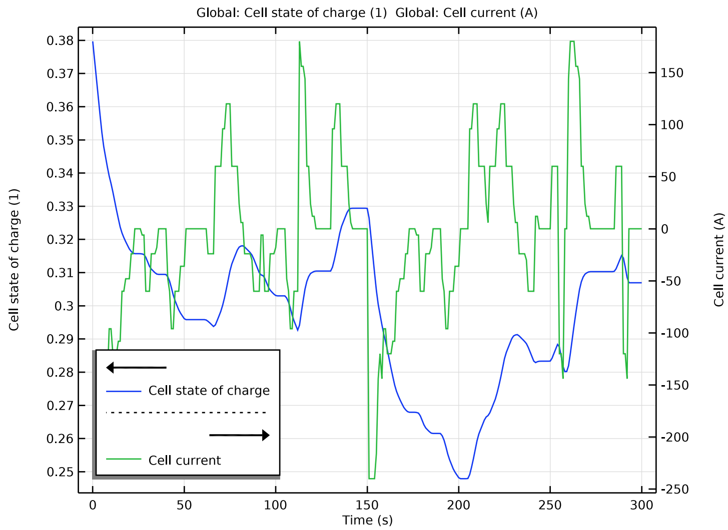
7 In the **Cell Voltage** toolbar, click **Plot**.



Cell State of Charge (lb)

Also a state of charge versus time plot was created by default:

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



Voltage Losses and Load

Proceed as follows to create a plot that compares the different voltage losses in the model:

1 In the **Results** toolbar, click **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Voltage Losses and Load` in the **Label** text field.

Global 1

1 Right-click **Voltage Losses and Load** 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** > **Overpotentials** > **lb.eta_ir - Ohmic overpotential - V**.

3 Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)** > **Lumped Battery** > **Overpotentials** > **lb.eta_act - Activation overpotential - V**.

4 Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)** > **Lumped Battery** > **Overpotentials** > **lb.eta_conc - Concentration overpotential - V**.

5 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

6 In the **Expression** text field, type `t`.

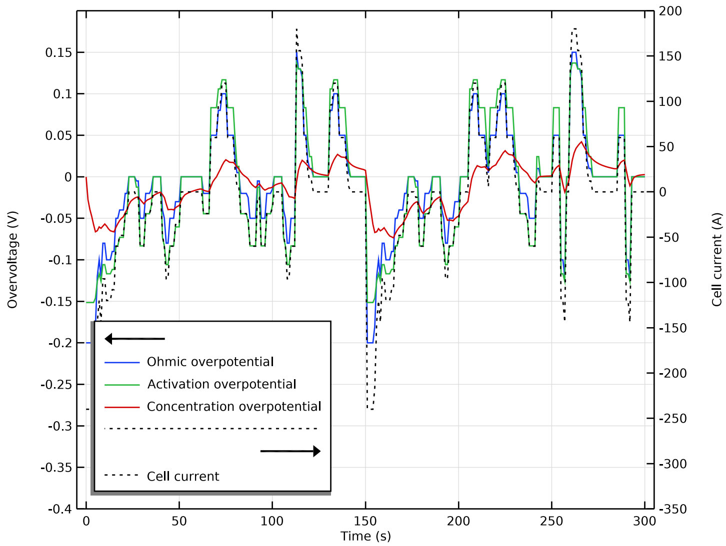
Global 2

1 In the **Model Builder** window, right-click **Voltage Losses and Load** 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.I_cell - Cell current - A**.
3 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.
4 In the **Expression** text field, type `t`.
5 Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dotted**.
6 From the **Color** list, choose **Black**.

Voltage Losses and Load

1 In the **Model Builder** window, click **Voltage Losses and Load**.
2 In the **Settings** window for **1D Plot Group**, locate the **Title** section.
3 From the **Title type** list, choose **None**.
4 Locate the **Plot Settings** section.
5 Select the **y-axis label** checkbox. In the associated text field, type `Overvoltage (V)`.
6 Select the **Two y-axes** checkbox.
7 In the table, select the **Plot on secondary y-axis** checkbox for **Global 2**.
8 Locate the **Axis** section. Select the **Manual axis limits** checkbox.
9 In the **x maximum** text field, type `305`.
10 In the **y minimum** text field, type `-0.4`.
11 In the **y maximum** text field, type `0.2`.
12 In the **Secondary y minimum** text field, type `-350`.
13 In the **Secondary y maximum** text field, type `200`.
14 Locate the **Legend** section. From the **Position** list, choose **Lower left**.

15 In the **Voltage Losses and Load** toolbar, click **Plot**.



LUMPED BATTERY (LB)

Voltage Losses 1

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

   Now change the default values for the voltage losses to use values defined in the **Parameters** node instead.
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. In the τ text field, type `tau`.

ROOT

The next step is to set up the optimization solver used for the parameter estimation. We will do this in a new study node.

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 the **Add Study** button in the window toolbar.

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

STUDY 2 - PARAMETER ESTIMATION

1 In the **Settings** window for **Study**, type `Study 2 - Parameter Estimation` in the **Label** text field.

2 Locate the **Study Settings** section. Clear the **Generate default plots** checkbox.

The first part of the tutorial is now complete. In the second part you will learn how to run an optimization solver to perform an estimation of the different voltage loss parameters.

Parameter Estimation

1 In the **Study** toolbar, click **Optimization** and choose **Parameter Estimation**.

The **Parameter Estimation** study step is used to construct the objective function that is to be minimized by the optimization solver. The objective function in this case will equal the sum of the squared differences between the modeled and the experimental cell voltages, for all stored times in the data.

2 In the **Settings** window for **Parameter Estimation**, locate the **Experimental Data** section.

3 From the **Data source** list, choose **Result table**.

Note that you can also import a data file directly here instead of using the table.

4 Locate the **Data Column Settings** section. In the table, enter the following settings:

Columns	Type	Settings
Time (s)	Time	Time unit=s
Voltage (V)	Value	Model expression=1, Name=col2, Weight=1
Current (A)	Ignored column	

5 In the table, click to select the cell at row number 2 and column number 3.

6 In the **Model expression** text field, type `comp1.lb.E_cell`.

The **Model expression** tells what value in the model the data corresponds to.

7 In the **Unit** text field, type `V`.

Now define what parameters (control variables) we should run the parameter estimation for:

8 Locate the **Estimated Parameters** section. Click + **Add** three times.

There should now be three control variables present in the table. In order to improve the optimization you need to provide suitable scales for these (the **Scale** column in the table).

9 In the table, enter the following settings:

Parameter name	Initial value	Scale	Lower bound	Upper bound
eta_IR_1C (Ohmic overpotential at 1C, fitting parameter)	`10[mV]`	`0.01`		
invJ0 (Inverse dimensionless charge exchange current, fitting parameter)	1	1		
tau (Diffusion time constant, fitting parameter)	`1000[s]`	1000		

The Lower/Upper bound columns are not used in this model. They may be used to put bounds on the control variables during the optimization.

The **Levenberg-Marquardt** is suitable for global least-squares problems.

10 Locate the **Parameter Estimation Method** section. Find the **Solver settings** subsection. From the **Least-squares time/parameter list method** list, choose **Use only least-squares data points**.

DEFINITIONS (COMP1)

Global Variable Probe 1 (var1)

By adding probes for the fitting parameters (the control variables) you can monitor how these change during the optimization.

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Definitions** and choose **Global Variable Probe**.

2 In the **Settings** window for **Global Variable Probe**, locate the **Expression** section.

3 In the **Expression** text field, type `eta_IR_1C`.

Global Variable Probe 2 (var2)

1 Right-click **Definitions** and choose **Global Variable Probe**.

2 In the **Settings** window for **Global Variable Probe**, locate the **Expression** section.

3 In the **Expression** text field, type `invJ0`.

Global Variable Probe 3 (var3)

1 Right-click **Definitions** and choose **Global Variable Probe**.

2 In the **Settings** window for **Global Variable Probe**, locate the **Expression** section.

3 In the **Expression** text field, type `tau`.

STUDY 2 - PARAMETER ESTIMATION

The parameter estimation problem is now ready for solving. Since the model will run multiple times in order to find the minimum of the objective function, this computation will take a little longer (about a minute) to run than the first study.

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

RESULTS

Change what data the plots are pointing to in order to plot the results of the parameter estimation study (Figure 1 and Figure 2).

Cell Voltage

1 In the **Model Builder** window, under **Results** click **Cell Voltage**.

2 In the **Settings** window for **1D Plot Group**, locate the **Data** section.

3 From the **Dataset** list, choose **Study 2 - Parameter Estimation/Solution 2 (sol2)**.

4 In the **Cell Voltage** toolbar, click **Plot**.

Voltage Losses and Load

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

2 In the **Settings** window for **1D Plot Group**, locate the **Data** section.

3 From the **Dataset** list, choose **Study 2 - Parameter Estimation/Solution 2 (sol2)**.

4 In the **Voltage Losses and Load** toolbar, click **Plot**.

STUDY 2 - PARAMETER ESTIMATION

The cell voltage plot can be set as output while solving to monitor the optimization process in the graphics window during computation.

Parameter Estimation

1 In the **Model Builder** window, under **Study 2 - Parameter Estimation** click **Parameter Estimation**.

2 In the **Settings** window for **Parameter Estimation**, click to expand the **Output While Solving** section.

3 Select the **Plot** checkbox.

You may now try to recompute the solution to see how the experimental and model cell voltage curves approach each other during optimization.

RESULTS

The second part of the tutorial is now complete. The final part is to set up a new study for cell voltage prediction. Note that the previous two studies used a 300 s load cycle data. For the prediction study, a full load cycle with additional 300 s will be used. First, we will import the full load cycle data consisting of the battery load and experimental cell voltage data as a table, as before, and use this table for defining time-dependent battery current and experimental voltage functions. (Note that the initial 300 s of the full load cycle data is exactly identical to the load cycle data imported for the previous study).

Full Load Cycle Data

1 In the **Results** toolbar, click **Table**.

2 In the **Settings** window for **Table**, type `Full Load Cycle Data` in the **Label** text field.

3 Locate the **Data** section. Click **Import**.

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

FULL LOAD CYCLE DATA

1 Go to the **Full Load Cycle Data** window.

This data file also contains three different columns: Time, Current and Voltage, as before.

DEFINITIONS (COMP1)

Interpolation - E and I vs. t (full)

1 In the **Definitions** toolbar, click **Interpolation**.

2 In the **Settings** window for **Interpolation**, type `Interpolation - E and I vs. t (full)` in the **Label** text field.

3 Locate the **Definition** section. From the **Data source** list, choose **Result table**.

4 From the **Table from** list, choose **Full Load Cycle Data**.

5 Locate the **Data Column Settings** section. In the table, click to select the cell at row number 1 and column number 1.

6 In the **Unit** text field, type `s`.

7 In the table, click to select the cell at row number 2 and column number 1.

8 In the **Name** text field, type `E_cell_exp_full`.

9 In the table, enter the following settings:

Columns	Type	Settings
Current (A)	Function values	Function name=I_cell_exp_full

10 In the **Name** text field, type `I_cell_exp_full`.

Variables 1

Next, we will define variables corresponding to the time-dependent battery current and the experimental cell voltage of the full load cycle. (The experimental cell voltage variable will only be used during postprocessing.)

Variables 2

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Definitions** right-click **Variables 1** and choose **Duplicate**.

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

3 In the table, enter the following settings:

Name	Expression	Unit	Description
`I_cell_exp`	`I_cell_exp_full(t)[A]`	A	`Experimental cell current - full load cycle`
`E_cell_exp`	`E_cell_exp_full(t)[V]`	V	`Experimental cell voltage - full load cycle`

ROOT

Add a new time-dependent study for prediction of the full 600 s load cycle. Modify the model configuration for this study step to disable **Variables1** (that consists of variables corresponding to the 300 s load cycle). Also, set up the study to use the optimized lumped parameter values from the previous parameter estimation study.

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 the **Add Study** button in the window toolbar.

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

STUDY 3 - FULL LOAD CURVE PREDICTION

In the **Settings** window for **Study**, type `Study 3 - Full Load Curve Prediction` in the **Label** text field.

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 3 - Full Load Curve Prediction** 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(0,1,600)`.

4 From the **Tolerance** list, choose **User controlled**.

5 In the **Relative tolerance** text field, type `0.001`.

6 Locate the **Physics and Variables Selection** section. Select the **Modify model configuration for study step** checkbox.

7 In the tree, select **Component 1 (comp1)** > **Definitions** > **Variables 1**.

8 Click **Disable**.

9 Click to expand the **Values of Dependent Variables** section. Find the **Initial values of variables solved for** subsection. From the **Settings** list, choose **User controlled**.

10 Find the **Values of variables not solved for** subsection. From the **Settings** list, choose **User controlled**.

11 From the **Method** list, choose **Solution**.

12 From the **Study** list, choose **Study 2 - Parameter Estimation, Time Dependent**.

13 In the **Model Builder** window, click **Study 3 - Full Load Curve Prediction**.

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

15 Clear the **Generate default plots** checkbox.

Before we compute the prediction study, it may be useful, for completeness, to update the model configuration for the previous two study steps to disable **Variables2** (that consists of variables corresponding to the 600 s full load cycle).

STUDY 1 - LOAD CURVE SIMULATION

1 In the **Model Builder** window, under **Study 1 - Load Curve Simulation** click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Physics and Variables Selection** section.

3 Select the **Modify model configuration for study step** checkbox.

4 In the tree, select **Component 1 (comp1)** > **Definitions** > **Variables 2**.

5 Click **Disable**.

STUDY 2 - PARAMETER ESTIMATION

1 In the **Model Builder** window, under **Study 2 - Parameter Estimation** click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Physics and Variables Selection** section.

3 Select the **Modify model configuration for study step** checkbox.

4 In the tree, select **Component 1 (comp1)** > **Definitions** > **Variables 2**.

5 Click **Disable**.

STUDY 3 - FULL LOAD CURVE PREDICTION

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

RESULTS

The results of the prediction study (Figure 3) can be plotted by duplicating the **Cell Voltage** figure.

Cell Voltage: Full Cycle Prediction

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

2 In the **Settings** window for **1D Plot Group**, type `Cell Voltage: Full Cycle Prediction` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 3 - Full Load Curve Prediction/Solution 3 (sol3)**.

4 Locate the **Axis** section. In the **x maximum** text field, type `610`.

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

Global 1

1 In the **Model Builder** window, expand the **Cell Voltage: Full Cycle Prediction** node, then click **Global 1**.

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

3 In the table, enter the following settings:

Expression	**Unit**	**Description**
`lb.E_cell`	`V`	`Predicted cell voltage`

4 In the **Cell Voltage: Full Cycle Prediction** toolbar, click **Plot**.

Global Evaluation: Standard Deviation (Study1)

Finally, you can set up global evaluations for calculating the standard deviation of the modeled cell voltage from the experimental values for all the three studies as follows:

1 In the **Results** toolbar, click **Global Evaluation**.

2 In the **Settings** window for **Global Evaluation**, type `Global Evaluation: Standard Deviation (Study1)` in the **Label** text field.

3 Locate the **Expressions** section. In the table, enter the following settings:

Expression	**Unit**	**Description**
`lb.E_cell-E_cell_exp`	`V`	

4 Locate the **Data Series Operation** section. From the **Transformation** list, choose **Standard deviation**.

5 Click **Evaluate**.

Global Evaluation: Standard Deviation (Study2)

1 Right-click **Global Evaluation: Standard Deviation (Study1)** and choose **Duplicate**.

2 In the **Settings** window for **Global Evaluation**, type `Global Evaluation: Standard Deviation (Study2)` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 2 - Parameter Estimation/Solution 2 (sol2)**.

4 Click **Evaluate**.

Global Evaluation: Standard Deviation (Study3)

1 Right-click **Global Evaluation: Standard Deviation (Study2)** and choose **Duplicate**.

2 In the **Settings** window for **Global Evaluation**, type `Global Evaluation: Standard Deviation (Study3)` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 3 - Full Load Curve Prediction/Solution 3 (sol3)**.

You can choose only the latter half of the full load cycle to obtain the standard deviation of the prediction study.

4 From the **Time selection** list, choose **Manual**.

5 In the **Time indices (1-601)** text field, type `range(302,1,601)`.

6 Click **= Evaluate**.