

Lithium-Ion Battery Internal Resistance

This tutorial analyzes the polarization (voltage) losses in a lithium-ion battery during a Hybrid Pulse Power Characterization (HPPC) test. The model is a continuation of the Lithium-Ion Battery Rate Capability tutorial, where the total discharge energy was compared between an energy-optimized and a power-optimized battery.

The internal resistance of a battery cell is generally calculated by dividing the voltage losses by the cell current. Many physical battery properties affect the internal resistance and rate capability, for instance:

- **•** the thicknesses of the electrodes and separator layers,
- **•** the porosity of the electrodes and separator layers,
- **•** the active material particle size in the electrodes,
- **•** the choice of active electrode material,
- **•** other material choices, for example, the electrolyte and electronic conductor, and
- the degree of lithiation of the electrode material due to several material properties being dependent on the intercalation state.

The internal resistance can typically be decreased by using thinner separator and electrode layers, higher porosities, and smaller active material particles. However, decreasing the internal resistance will often also mean decreasing the capacity of the battery, if the amount of electrode material per total battery cell volume decreases.

The choice of active materials are important as well. Some materials are able to shift their lithium concentration efficiently even at high current loads. Additionally, the electrolyte is also important; for example, polymer batteries are seldom used in power applications since these contain a nonliquid electrolyte with poor lithium-ion transport properties.

Model Definition

The model is set up in 1D for a graphite/NMC battery cell. A more detailed description of the model can be found in Lithium-Ion Battery Base Model in 1D.

In this tutorial we will investigate the internal resistance of a $21,700$ battery where it is assumed that 90% of the internal volume is occupied by the active jelly roll (electrode, separator, and current collector layers). The battery is subjected to a 10 A discharge pulse for 10 s, followed by a 20 s rest, followed by a 10 A charge for 10 s. The internal resistance and associated polarization losses are analyzed both for an energy optimized and a power optimized cell, featuring a cross-sectional cell capacity of 40 Ah/m² and 20 Ah/m², respectively. The battery model is parameterized in such a way that when changing the cell capacity, the electrode layer thicknesses change correspondingly.

Due to the 1D geometry, the current load of the battery model is formulated as a current density boundary condition with the unit of A/m^2 . To convert from the cell current I_{cell} (A) to the applied current density $i_{\text{app}} (A/m^2)$ on the jelly roll we first compute the cell area as

$$
A_{\text{cell}} = \frac{V_{\text{cell}}}{L_{\text{cell}}} \tag{1}
$$

where the length L_{cell} of the cell is calculated as

$$
L_{\text{cell}} = L_{\text{neg}} + L_{\text{sep}} + L_{\text{pos}} + L_{\text{ccs}}/2
$$
 (2)

where L_{ccs} is the sum both thickness of the positive and negative current collector foils in jelly roll. (The factor $1/2$ stems from the configuration of a typical jelly roll where each metal foil is being coated on both sides by the same electrode layer.)

The applied current density, used as a boundary condition in the 1D model, is then defined as

$$
i_{\rm app} = \frac{I_{\rm cell}}{A_{\rm cell}}\tag{3}
$$

The Events interface is used to define a duration-based state variable *S*ch-dch attaining the values -1, 0, or 1, corresponding to discharge, rest, or charge during the simulation, respectively.

The boundary condition at the positive electrode current collector boundary is finally defined as

$$
i_s = S_{\text{ch-dch}} i_{\text{app}} \tag{4}
$$

(Instead of using Events and a state variable, one could also have formulated the boundary condition using a time-dependent function as in the 1D Lithium-Ion Battery Drive-Cycle Monitoring tutorial. The use of Events however improves the numerical performance of the model since the fast transitions between charge and discharge need not the be resolved by the time-dependent solver.)

ANALYZING VOLTAGE LOSSES

Various quantities can be computed in order to analyze the voltage losses of a physicsbased lithium-ion battery model.

General for an analysis of this kind is that we want to compare the computed cell voltage to the open circuit voltage, which is a function of the (average) degrees of lithiation of the electrodes. For both the negative and the positive electrode the average degrees of lithiation, $sol_{\text{avg}}(1)$, can be computed by first integrating over the extra dimension in the radial direction of the electrode particles, and then by a second integration over the whole electrode domain. The OCV of the cell may then be computed as

$$
E_{\text{OCV,cell}} = E_{\text{eq,pos}}(\text{sol}_{\text{avg, pos}}) - E_{\text{eq,neg}}(\text{sol}_{\text{avg, neg}})
$$
(5)

The total polarization of the cell is then computed as

$$
E_{\text{pol, tot}} = E_{\text{cell}} - E_{\text{OCV,cell}} \tag{6}
$$

The internal resistance is obtained by dividing by the cell current

$$
R_{\text{cell}} = \frac{E_{\text{pol, tot}}}{I_{\text{cell}}} \tag{7}
$$

For the voltage losses attributed to separate physical phenomena, we will define a set of voltage loss variables that fulfill the relation

$$
E_{\text{pol, tot}} = E_l + E_s + E_{\text{act}} + E_{\text{conc}} \tag{8}
$$

where the above variables represent the electrolyte ohmic, electrode ohmic, activation, and concentration voltage losses (V), respectively.

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The general approach to define the above loss variables is to first compute the total loss in terms of electrical power, and then to divide this number by the cell current (see also [Ref. 1](#page-9-0)).

The ohmic losses are computed by integrating the dot product of the gradient of the potential and the corresponding current vector, resulting in

$$
E_{l} = \frac{\int -\nabla \phi_{l} \cdot \mathbf{i}_{l} \partial \Omega}{I_{\text{cell}}} \tag{9}
$$

and

$$
E_s = \frac{\int -\nabla \phi_s \cdot \mathbf{i}_s \partial \Omega}{I_{\text{cell}}} \tag{10}
$$

for the electrolyte and electrode phases, respectively. In the above and following integral expressions, the integration is made for all applicable domains, and Ω is the volume element.

For the activation losses due to the charge transfer reactions in the electrodes, the loss of electric power is computed by integrating the product of the activation overpotential and the volumetric current density

$$
E_{\rm act} = \frac{\int \eta i_v \partial \Omega}{I_{\rm cell}} \tag{11}
$$

Finally, the concentration losses are calculated by integrating the loss of electric power in charge transfer due to concentration gradients in the cell. This is computed as

$$
E_{\text{conc}} = \frac{\int \eta_{\text{conc}} i_v \partial \Omega}{I_{\text{cell}}} \tag{12}
$$

where the concentration overpotential is calculated as the difference between the local equilibrium potential of the charge transfer reaction at the surface of the electrode particles and the open circuit equilibrium potential of the whole electrode

$$
\eta_{\text{conc}} = E_{\text{eq}}(\text{sol}_{\text{surface}}) - E_{\text{eq}}(\text{sol}_{\text{avg}})
$$
(13)

where sol_{surface} is evaluated at the surface of the electrode particles, locally in the electrode.

[Figure 2](#page-5-0) shows the cell voltage and corresponding C-rates for the two cell configurations. The C-rates are slightly higher for the power-optimized (20 Ah/m^2) battery compared to the energy-optimized (40 Ah/m²) battery. The reason for this is that total current and volume are fixed, in combination with the energy-optimized featuring a higher capacity. The polarization (voltage deviation from the rest voltage) is however still higher for energy-optimized cell, despite the slightly lower C-rate.

Figure 2: Cell voltage and current C-rates versus time.

Dividing the polarization voltage by the current results in the internal resistance [\(Equation 7](#page-3-0)), which is shown in [Figure 3](#page-6-0). The resistance values are significantly higher for the energy optimized cell. The resistance increases with time, but is fairly similar for the two pulses.

Figure 3: Internal resistance versus time.

For a more detailed analysis of the origin of the different voltage losses, [Figure 4](#page-7-0) shows the total polarization of each domain, (that is, where [Equation 8](#page-3-1) has been computed separately per domain). Interestingly, the power-optimized cell features lower voltage losses in the electrodes, but higher losses in the separator, compared to the energyoptimized cell. The differences in the separator losses are directly attributed to the lower C-rate for the energy-optimized cell. All voltage losses increase with time during a pulse, but the positive losses seem to increase the most.

Figure 4: Voltage losses in the different domains versus time.

Finally, [Figure 5a](#page-8-0)nd [Figure 6](#page-8-1) show the voltage losses attributed to the different physical phenomena ([Equation 9](#page-4-0) to [Equation 12\)](#page-4-1) in the negative and positive electrodes, respectively. As expected, the power-optimized cell generally features lower voltage losses, except for the concentration overpotentials in the positive electrode where the losses for the energy-optimized cell are slightly lower, once again due to the slightly lower C-rate. All losses increase with time, but the electrolyte ohmic losses seem to affected the most. This is due to the changed electrolyte conductivity due to ion accumulation/depletion in the electrodes, and also due to a reaction from moving into the electrode gradually increasing the transport length for the ions.

Figure 5: Voltage losses in the negative graphite electrode.

Figure 6: Voltage losses in the positive NMC electrode.

Reference

1. A. Nyman, T.G. Zavalis, R. Elger, M. Behm, and G. Lindbergh, "Analysis of the Polarization in Li-Ion Battery Cell by Numerical Simulations," *J. Electrochem. Soc.*, vol. 157, no. 11, pp. A1236–A1246, 2010.

Application Library path: Battery_Design_Module/Batteries,_Lithium-Ion/ li_battery_internal_resistance

Modeling Instructions

APPLICATION LIBRARIES

- **1** From the **File** menu, choose **Application Libraries**.
- **2** In the **Application Libraries** window, select **Battery Design Module>Batteries, Lithium-Ion> lib_base_model_1d** in the tree.
- **3** Click **o** Open.

In this tutorial we will perform a HPPC (hybrid pulse power characterization) test on the battery model you just loaded. The combined discharge-rest-charge load profile will be applied at 50% state of charge.

GLOBAL DEFINITIONS

Parameters 1

- **1** In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.
- **2** In the **Settings** window for **Parameters**, locate the **Parameters** section.
- **3** In the table, enter the following settings:

Parameters - Pulse and Cell Area

Add a second group of parameters from a text file.

- **1** In the **Home** toolbar, click **P**^{*i*} Parameters</sub> and choose Add>Parameters.
- **2** In the **Settings** window for **Parameters**, type Parameters Pulse and Cell Area in the **Label** text field.
- **3** Locate the **Parameters** section. Click **Load from File**.
- **4** Browse to the model's Application Libraries folder and double-click the file li battery internal resistance parameters.txt.

ADD PHYSICS

- **1** In the **Home** toolbar, click **Add Physics** to open the **Add Physics** window.
- **2** Go to the **Add Physics** window.

To construct the current density boundary condition we will make use of a discrete state variable, set up by the Events interface.

- **3** In the tree, select **Mathematics>ODE and DAE Interfaces>Events (ev)**.
- **4** Click **Add to Component 1** in the window toolbar.
- **5** In the **Home** toolbar, click **Add Physics** to close the **Add Physics** window.

EVENTS (EV)

Discrete States 1

- **1** Right-click **Component 1 (comp1)>Events (ev)** and choose **Discrete States**.
- **2** In the **Settings** window for **Discrete States**, locate the **Discrete States** section.
- **3** In the table, enter the following settings:

The initial value of the state variable is -1, defining the discharge part of the load profile.

Event Sequence 1

Add a sequence to control the charge-to-rest and rest-to-discharge transitions.

In the **Physics** toolbar, click **Global** and choose **Event Sequence**.

Sequence Member 1

- **1** In the **Model Builder** window, expand the **Event Sequence 1** node, then click **Sequence Member 1**.
- **2** In the **Settings** window for **Sequence Member**, locate the **Sequence Member** section.
- **3** In the **Discrete state name** text field, type DCH.
- **4** From the **End condition** list, choose **Duration**.
- **5** In the **Duration** text field, type t_pulse.

6 Locate the **Reinitialization** section. In the table, enter the following settings:

Event Sequence 1

In the **Model Builder** window, click **Event Sequence 1**.

Sequence Member 2

- **1** In the **Physics** toolbar, click **Attributes** and choose **Sequence Member**.
- **2** In the **Settings** window for **Sequence Member**, locate the **Sequence Member** section.
- **3** In the **Discrete state name** text field, type REST.
- **4** From the **End condition** list, choose **Duration**.
- **5** In the **Duration** text field, type t_rest.
- **6** Locate the **Reinitialization** section. In the table, enter the following settings:

DEFINITIONS (COMP1)

Variables 1

Now add a current density variable based on the state variable, and a variable for the internal resistance.

- **1** In the **Model Builder** window, expand the **Component 1 (comp1)>Definitions** node, then click **Variables 1**.
- **2** In the **Settings** window for **Variables**, locate the **Variables** section.
- **3** In the table, enter the following settings:

LITHIUM-ION BATTERY (LIION)

Electrode Current Density 1

- **1** In the **Model Builder** window, expand the **Component 1 (comp1)>Lithium-Ion Battery (liion)** node, then click **Electrode Current Density 1**.
- **2** In the **Settings** window for **Electrode Current Density**, locate the **Electrode Current Density** section.
- **3** In the $i_{n,s}$ text field, type I app.

STUDY 1

Step 1: Time Dependent

Specify the duration of the simulation and the times of interest to store in the solution in the times list.

1 In the **Model Builder** window, expand the **Study 1** node, then click

Step 1: Time Dependent.

- **2** In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.
- **3** From the **Time unit** list, choose **s**.
- **4** In the **Output times** text field, type range(0,t_pulse/10,2*t_pulse+t_rest).

Add a parametric sweep varying the cross-sectional cell capacity parameter. This will perform the HPPC simulation both for a power optimized and an energy-optimized battery. When varying the q_cell parameter, also the thickness of the electrodes will be updated. These correlations are defined in the **Parameters 1** node.

Parametric Sweep

- **1** In the **Study** toolbar, click $\frac{1}{2}$ **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:

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

RESULTS

Plot the cell voltage and current as follows:

Cell Voltage and Current

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

Global 1

- Right-click **Cell Voltage and Current** and choose **Global**.
- 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>C_rate - C rate**.
- Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.
- From the **Color** list, choose **Cycle (reset)**.
- Click to expand the **Legends** section.

Point Graph 1

- In the **Model Builder** window, click **Point Graph 1**.
- In the **Settings** window for **Point Graph**, click to expand the **Legends** section.
- Select the **Show legends** check box.
- Find the **Include** subsection. Clear the **Point** check box.
- Find the **Prefix and suffix** subsection. In the **Suffix** text field, type , E_cell.

Cell Voltage and Current

- In the **Model Builder** window, click **Cell Voltage and Current**.
- In the **Settings** window for **1D Plot Group**, click to expand the **Title** section.
- From the **Title type** list, choose **None**.
- Locate the **Plot Settings** section. Select the **Two y-axes** check box.
- In the table, select the **Plot on secondary y-axis** check box for **Global 1**.
- Locate the **Legend** section. From the **Position** list, choose **Upper left**.

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

Internal Resistance

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

Plot the internal resistance as follows:

- **2** In the **Settings** window for **1D Plot Group**, type Internal Resistance in the **Label** text field.
- **3** Locate the **Data** section. From the **Dataset** list, choose **Study 1/ Parametric Solutions 1 (sol2)**.

Global 1

- **1** Right-click **Internal Resistance** 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)>Definitions> Variables>R_internal - R_internal -** .
- **3** Locate the **Legends** section. Find the **Include** subsection. Clear the **Description** check box.

Internal Resistance

- **1** In the **Model Builder** window, click **Internal Resistance**.
- **2** In the **Settings** window for **1D Plot Group**, locate the **Title** section.
- **3** From the **Title type** list, choose **None**.
- **4** Locate the **Legend** section. From the **Position** list, choose **Upper middle**.

5 In the **Internal Resistance** toolbar, click **Plot**.

DEFINITIONS (COMP1)

Add an additional list of variables, to be used for postprocessing, from a text file.

Variables 2

- **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 li_battery_internal_resistance_variables.txt.

Many of the imported variables are marked in orange, indicating missing operators. Add these missing operators as follows:

Integration 1 (intop1)

- **1** In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **Integration**.
- **2** In the **Settings** window for **Integration**, type intop_neg in the **Operator name** text field.
- **3** Locate the **Source Selection** section. From the **Selection** list, choose **Negative Electrode**.

Integration 2 (intop2)

1 In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **Integration**.

- **2** In the **Settings** window for **Integration**, type intop_sep in the **Operator name** text field.
- **3** Locate the **Source Selection** section. From the **Selection** list, choose **Separator**.

Integration 3 (intop3)

- **1** In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **Integration**.
- **2** In the **Settings** window for **Integration**, type intop_pos in the **Operator name** text field.
- **3** Locate the **Source Selection** section. From the **Selection** list, choose **Positive Electrode**.

Variables 2

The variable expressions should now all have turned black.

STUDY 1

Update the solution to make the new variable definitions available in the already existing solution.

1 In the **Study** toolbar, click **Update Solution**.

RESULTS

Voltage Losses, All Domains

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

Plot the voltage losses in each domain as follows:

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

Global 1

- **1** Right-click **Voltage Losses, All Domains** and choose **Global**.
- **2** In the **Settings** window for **Global**, locate the **Data** section.
- **3** From the **Dataset** list, choose **Study 1/Parametric Solutions 1 (sol2)**.
- **4** From the **Parameter selection (q_cell)** list, choose **From list**.
- **5** In the **Parameter values (q_cell (A*h/m^2))** list, select **20**.
- **6** Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Definitions>Variables>E_neg - Voltage loss, negative - V**.
- **7** Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Definitions>Variables>E_sep - Voltage loss, separator - V**.
- Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Definitions>Variables>E_pos - Voltage loss, positive - V**.
- Locate the **Legends** section. Find the **Include** subsection. Clear the **Solution** check box.
- Clear the **Description** check box.
- Select the **Expression** check box.

Global 2

- Right-click **Global 1** and choose **Duplicate**.
- In the **Settings** window for **Global**, locate the **Data** section.
- In the **Parameter values (q_cell (A*h/m^2))** list, select **40**.
- Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.
- From the **Color** list, choose **Cycle (reset)**.
- Locate the **Legends** section. Clear the **Show legends** check box.

Voltage Losses, All Domains

- In the **Model Builder** window, click **Voltage Losses, All Domains**.
- In the **Settings** window for **1D Plot Group**, locate the **Title** section.
- From the **Title type** list, choose **Manual**.
- In the **Title** text area, type Solid Lines: Power optimized cell, Dashed Lines: Energy optimized cell.
- Locate the **Plot Settings** section.
- Select the **y-axis label** check box. In the associated text field, type Voltage (V).
- Locate the **Legend** section. From the **Position** list, choose **Upper left**.

8 In the **Voltage Losses, All Domains** toolbar, click **Plot**.

Plot the individual voltage losses, stemming from different phenomena, in the negative electrode as follows:

Voltage Losses, Negative Electrode

- **1** In the Home toolbar, click **Add Plot Group** and choose **1D Plot Group**.
- **2** In the **Settings** window for **1D Plot Group**, type Voltage Losses, Negative Electrode in the **Label** text field.

Global 1

- **1** Right-click **Voltage Losses, Negative Electrode** and choose **Global**.
- **2** In the **Settings** window for **Global**, locate the **Data** section.
- **3** From the **Dataset** list, choose **Study 1/Parametric Solutions 1 (sol2)**.
- **4** From the **Parameter selection (q_cell)** list, choose **From list**.
- **5** In the **Parameter values (q_cell (A*h/m^2))** list, select **20**.
- **6** Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Definitions>Variables>E_s_neg - Electrode ohmic voltage loss, negative - V**.
- **7** Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Definitions>Variables>E_l_neg - Electrolyte ohmic voltage loss, negative - V**.
- Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Definitions>Variables>E_act_neg - Electrode activation voltage loss, negative - V**.
- Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Definitions>Variables>E_conc_neg - Concentration voltage loss, negative - V**.
- In the **Voltage Losses, Negative Electrode** toolbar, click **Plot**.
- Locate the **Legends** section. Find the **Include** subsection. Clear the **Solution** check box.
- Clear the **Description** check box.
- Select the **Expression** check box.

Global 2

- Right-click **Global 1** and choose **Duplicate**.
- In the **Settings** window for **Global**, locate the **Data** section.
- In the **Parameter values (q_cell (A*h/m^2))** list, select **40**.
- Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.
- From the **Color** list, choose **Cycle (reset)**.
- Locate the **Legends** section. Clear the **Show legends** check box.

Voltage Losses, Negative Electrode

- In the **Model Builder** window, click **Voltage Losses, Negative Electrode**.
- In the **Settings** window for **1D Plot Group**, locate the **Plot Settings** section.
- Select the **y-axis label** check box. In the associated text field, type Voltage (V).
- Locate the **Title** section. From the **Title type** list, choose **Manual**.
- In the **Title** text area, type Solid Lines: Power optimized cell, Dashed Lines: Energy optimized cell.
- Locate the **Legend** section. From the **Position** list, choose **Upper left**.

7 In the **Voltage Losses, Negative Electrode** toolbar, click **Plot**.

Duplicate and modify the plot to show the corresponding values for the positive electrode.

Voltage Losses, Positive Electrode

- **1** Right-click **Voltage Losses, Negative Electrode** and choose **Duplicate**.
- **2** In the **Settings** window for **1D Plot Group**, type Voltage Losses, Positive Electrode in the **Label** text field.

Global 1

- **1** In the **Model Builder** window, expand the **Voltage Losses, Positive Electrode** 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:

Global 2

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

- **2** In the **Settings** window for **Global**, locate the **y-Axis Data** section.
- **3** In the table, enter the following settings:

Voltage Losses, Positive Electrode

- **1** In the **Model Builder** window, click **Voltage Losses, Positive Electrode**.
- 2 In the **Voltage Losses, Positive Electrode** toolbar, click **Plot**.

