

Lithium-Ion Battery Internal Resistance

Introduction

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_{app} (A/m²) 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, $sol_{avg}(1)$, 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

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

The internal resistance is obtained by dividing by the cell current

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

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

$$E_{\text{pol, tot}} = E_l + E_s + E_{\text{act}} + E_{\text{conc}}$$
(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).

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

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

and

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

$$E_{\rm conc} = \frac{\int \eta_{\rm conc} i_v \partial \Omega}{I_{\rm cell}}$$
(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

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

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

Figure 2 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/m^2) 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), which is shown in Figure 3. 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 shows the total polarization of each domain, (that is, where Equation 8 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 energy-optimized 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 5 and Figure 6 show the voltage losses attributed to the different physical phenomena (Equation 9 to Equation 12) 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

- I From the File menu, choose Application Libraries.
- 2 In the Application Libraries window, select Battery Design Module>Batteries, Lithium-Ion> lib_base_model_Id in the tree.
- 3 Click < 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

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

Name	Expression	Value	Description
soc_init	50[%]	0.5	Initial SOC

Parameters - Pulse and Cell Area

Add a second group of parameters from a text file.

- I In the Home toolbar, click P; Parameters 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

- I 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 I in the window toolbar.
- 5 In the Home toolbar, click 🙀 Add Physics to close the Add Physics window.

EVENTS (EV)

Discrete States 1

- I Right-click Component I (compl)>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:

Name	Initial value (u0)	Description
CH_DCH	- 1	State variable (=-1 for discharge, =0 for rest, =+1 for charge)

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

- I In the Model Builder window, expand the Event Sequence I node, then click Sequence Member I.
- 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:

Variable	Expression
CH_DCH	0

Event Sequence 1

In the Model Builder window, click Event Sequence I.

Sequence Member 2

- I 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:

Variable	Expression
CH_DCH	1

DEFINITIONS (COMPI)

Variables I

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

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

Name	Expression	Unit	Description
I_app	I_pulse/A_cell*CH_DCH	A/m²	Applied current density
R_internal	<pre>E_pol_tot/(I_app*A_cell)</pre>	Ω	R_internal
C_rate	I_app/I_1C		C rate

LITHIUM-ION BATTERY (LIION)

Electrode Current Density 1

- I In the Model Builder window, expand the Component I (compl)>Lithium-Ion Battery (liion) node, then click Electrode Current Density I.
- **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 I

Step 1: Time Dependent

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

- I In the Model Builder window, expand the Study I node, then click Step I: 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 I** node.

Parametric Sweep

- I 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
q_cell (Cross-sectional cell capacity)	20 40	A*h/m^2

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 **ID Plot Group**, type Cell Voltage and Current in the **Label** text field.

Global I

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

Point Graph 1

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

Cell Voltage and Current

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



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

Internal Resistance

I In the Home toolbar, click 🚛 Add Plot Group and choose ID Plot Group.

Plot the internal resistance as follows:

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

Global I

- I 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 I (compl)>Definitions> Variables>R_internal Ω.
- 3 Locate the Legends section. Find the Include subsection. Clear the Description check box.

Internal Resistance

- I In the Model Builder window, click Internal Resistance.
- 2 In the Settings window for ID 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 **O Plot**.

DEFINITIONS (COMPI)

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

Variables 2

- I In the Model Builder window, under Component I (compl) 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)

- I 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)

I 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)

- I 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 I

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

I In the Study toolbar, click *C* Update Solution.

RESULTS

Voltage Losses, All Domains

I In the Home toolbar, click 🚛 Add Plot Group and choose ID Plot Group.

Plot the voltage losses in each domain as follows:

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

Global I

- I 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 I/Parametric Solutions I (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 I (compl)>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 I (comp1)>Definitions>Variables>E_sep Voltage loss, separator V.

- 8 Click Add Expression in the upper-right corner of the y-Axis Data section. From the menu, choose Component I (compl)>Definitions>Variables>E_pos Voltage loss, positive V.
- 9 Locate the Legends section. Find the Include subsection. Clear the Solution check box.
- **IO** Clear the **Description** check box.
- II Select the Expression check box.

Global 2

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

Voltage Losses, All Domains

- I In the Model Builder window, click Voltage Losses, All Domains.
- 2 In the Settings window for ID Plot Group, locate the Title section.
- **3** From the **Title type** list, choose **Manual**.
- **4** In the **Title** text area, type Solid Lines: Power optimized cell, Dashed Lines: Energy optimized cell.
- 5 Locate the Plot Settings section.
- 6 Select the y-axis label check box. In the associated text field, type Voltage (V).
- 7 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

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

Global I

- I 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 I/Parametric Solutions I (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 I (compl)>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 I (compl)>Definitions>Variables>E_l_neg Electrolyte ohmic voltage loss, negative V.

- 8 Click Add Expression in the upper-right corner of the y-Axis Data section. From the menu, choose Component I (compl)>Definitions>Variables>E_act_neg Electrode activation voltage loss, negative V.
- 9 Click Add Expression in the upper-right corner of the y-Axis Data section. From the menu, choose Component I (compl)>Definitions>Variables>E_conc_neg Concentration voltage loss, negative V.
- **IO** In the **Voltage Losses, Negative Electrode** toolbar, click **O** Plot.
- II Locate the Legends section. Find the Include subsection. Clear the Solution check box.
- **12** Clear the **Description** check box.
- **I3** Select the **Expression** check box.

Global 2

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

Voltage Losses, Negative Electrode

- I In the Model Builder window, click Voltage Losses, Negative Electrode.
- 2 In the Settings window for ID Plot Group, locate the Plot Settings section.
- **3** Select the **y-axis label** check box. In the associated text field, type Voltage (V).
- 4 Locate the Title section. From the Title type list, choose Manual.
- 5 In the Title text area, type Solid Lines: Power optimized cell, Dashed Lines: Energy optimized cell.
- 6 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

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

Global I

- I In the Model Builder window, expand the Voltage Losses, Positive Electrode node, then click Global I.
- 2 In the Settings window for Global, locate the y-Axis Data section.
- **3** In the table, enter the following settings:

Expression	Unit	Description
E_s_pos	V	Electrode ohmic voltage loss, positive
E_l_pos	V	Electrolyte ohmic voltage loss, positive
E_act_pos	V	Electrode activation voltage loss, positive
E_conc_pos	V	Concentration voltage loss, positive

Global 2

I 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:

Expression	Unit	Description
E_s_pos	V	Electrode ohmic voltage loss, positive
E_l_pos	V	Electrolyte ohmic voltage loss, positive
E_act_pos	V	Electrode activation voltage loss, positive
E_conc_pos	V	Particle concentration voltage loss, positive

Voltage Losses, Positive Electrode

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

