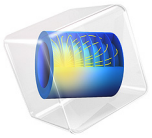

Single Particle Model of a Lithium-Ion Battery

Introduction

The single particle model for a lithium-ion battery is a simplification of the 1D model formulation (see the 1D Isothermal Lithium-Ion Battery model example), subject to a few assumptions. This model example demonstrates the Single Particle Battery interface for studying the discharge of a lithium-ion battery. The model is isothermal and is set in 0D space dimension. The voltage profiles are compared with the corresponding 1D formulation for a range of discharge currents.

In the single particle model formulation (Ref. 1and Ref. 2), the local potential and concentration gradients in the solution (electrolyte) phase are ignored and accounted for using a lumped solution resistance term. Similarly, the potential gradients in the solid phase of the electrodes are also neglected. Additionally, the porous electrode is treated as a large number of single particles all of them being subjected to the same conditions, since the reaction current distribution across the porous electrodes is assumed to be uniform. The single particle formulation accounts for solid diffusion in the electrode particles and the intercalation reaction kinetics.

The assumptions in the single particle formulation are typically valid for low-medium applied current densities. Additionally, the validity of the assumptions and the applicability of the model also depends on the parameters values and electrode-electrolyte chemistry used in the model. For example, the assumptions would be reasonable for thin electrodes, highly conductive electrodes, and so forth.

The single particle model formulation can be used for parameter estimation studies (kinetic and transport parameters) by comparing with experimental data. Additionally, it can be used instead of the more elaborate 1D formulation in computationally expensive scenarios such as thermal simulations, cycling behavior, battery pack simulations, and so forth.

Model Definition

The Single Particle Battery interface accounts for solid diffusion in the electrode particles and the intercalation reaction kinetics. The ohmic potential drop in the electrolyte is included using a lumped solution resistance term.

In this model example, the intercalation particles in the porous electrode are assumed to be spherical particles of identical size. Diffusion of lithium in the active material particles in the positive and negative electrodes is described by Fick's second law. The intercalation reaction kinetics is expressed using the lithium insertion kinetics.

This model example is set in 0D space dimension for studying a galvanostatic operation for different discharge currents ranging from 0.1 C to 2 C, and a charge-discharge cycling operation at 1 C. The cell capacity is specified though fractional volumes of the positive and negative electrodes in the battery. The individual electrode operational state-of-charges are used to specify the initial charge distribution in the battery.

MODEL PARAMETERS

All the model parameters required by the single particle model are identical to the parameters used in the 1D Isothermal Lithium-Ion Battery model, for the purpose of comparison of the discharge voltage profiles between the two formulations.

STUDY SETTINGS

Time Dependent with Initialization study is used in this model. This solves for the current distribution initialization study step followed by the time dependent study step.

Note that when computing the studies in the model file available in Application Libraries, Study 1 requires that the operation mode is set to Galvanostatic at the Single Particle Battery interface level and Study 2 requires that the operation mode is set to Charge-discharge cycling at the Single Particle Battery interface level.

Results and Discussion

The discharge curves from the single particle model are compared with the corresponding discharge profiles from the 1D model (1D Isothermal Lithium-Ion Battery). Note that the discharge data from the 1D model is imported as text files for the purpose of comparison. The parameter representing the electrolyte solution resistance R_{sol} would depend on temperature and applied current. In this model, a single value for the electrolyte solution resistance R_{sol} gives a reasonable comparison of the single particle model with the 1D model for the range of discharge currents simulated.

Figure 1 shows the comparison of the discharge voltage profiles from the single particle model and 1D model at discharge rates of 0.1 C, 1 C and 2 C, respectively.

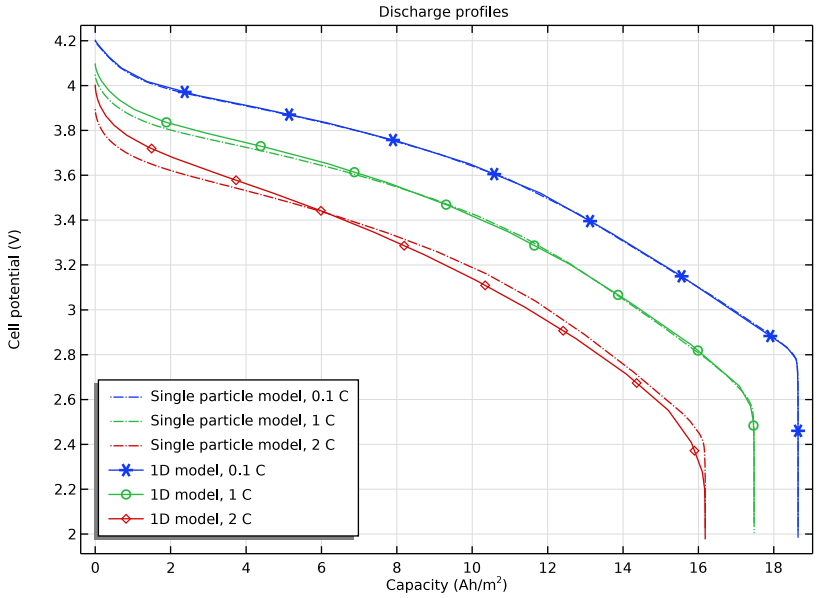

Figure 1: Single particle model compared to the 1D model at 0.1C, 1C and 2C.

Figure 1 shows that the single particle model reproduces the discharge curves for the 1D model fairly well. For higher discharge currents the deviations are larger. This is expected since at higher discharge currents the electrolyte transport limitations and potential drops result in an uneven reaction current density distribution over the porous electrodes, and the single particle assumption becomes less accurate. However, the electrolyte solution resistance R_{sol} could be set up as a function of the applied current in order to provide a better representation even at higher values of the discharge current.

Figure 2 shows a similar comparison of the charge-discharge cycling voltage profile from the single particle model and 1D model at an applied current of 1 C.

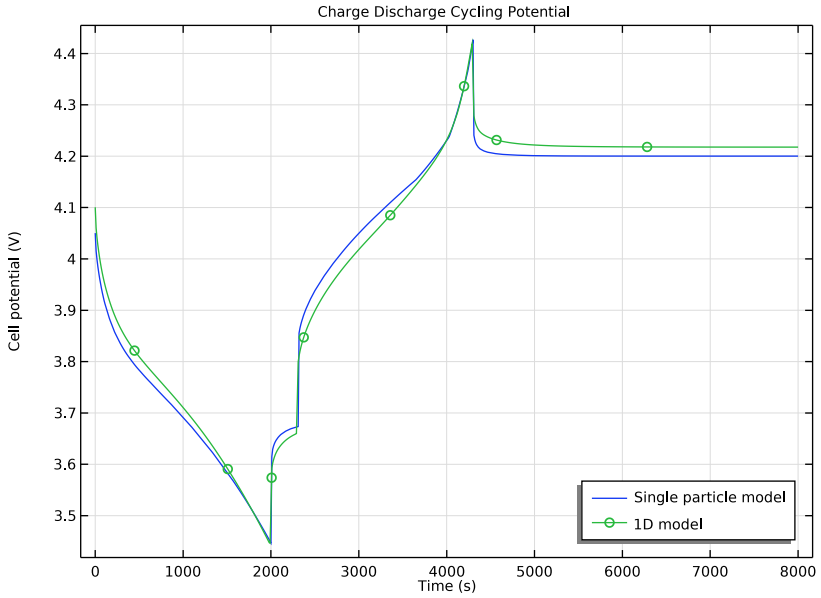

Figure 2: Single particle model compared to the 1D model for a charge-discharge cycling operation at 1C.

References

1. S. Santhanagopalan, Q. Guo, P. Ramadass, and R.E. White, "Review of Models for Predicting the Cycling Performance of Lithium Ion Batteries," *J. Power Sources*, vol. 156, no. 2, pp. 620–628, 2006.

2. M. Guo, G. Sikha, and R.E. White, "Single Particle Model for a Lithium Ion Cell: Thermal Behavior," *J. Electrochem. Soc.*, vol. 158, no. 2, pp. A122–A132, 2011.

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

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>Single Particle Battery (spb)**.
3. Click **Add**.
4. Click **Study**.
5. In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces> Time Dependent with Initialization**.
6. Click **Done**.

GLOBAL DEFINITIONS

Load the model parameters from a text file.

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. Click **Load from File**.
4. Browse to the model's Application Libraries folder and double-click the file `li_battery_single_particle_parameters.txt`.

Interpolation 1 (int1)

This model uses an interpolation function, imported from a text file, for the equilibrium potential of the negative electrode.

1. In the **Home** toolbar, click **Functions** and choose **Global>Interpolation**.
2. In the **Settings** window for **Interpolation**, locate the **Definition** section.
3. In the **Function name** text field, type `Eeq_neg`.
4. Click **Load from File**.
5. Browse to the model's Application Libraries folder and double-click the file `li_battery_1d_Eeq_neg.txt`.

6 Locate the **Interpolation and Extrapolation** section. From the **Interpolation** list, choose **Cubic spline**.

7 From the **Extrapolation** list, choose **Nearest function**.

8 Locate the **Units** section. In the **Function** table, enter the following settings:

Function	Unit
Eeq_neg	V

ADD MATERIAL

This model uses a positive electrode battery material from the material library.

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

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

3 In the tree, select **Battery>Electrodes>LMO, LiMn2O4 Spinel (Positive, Li-ion Battery)**.

4 Click the right end of the **Add to Component** split button in the window toolbar.

5 From the menu, choose **Add to Global Materials**.

6 In the **Home** toolbar, click **Add Material** to close the **Add Material** window.

DEFINITIONS (COMP1)

Load the model variables from a text file.

Variables 1

1 In the **Home** toolbar, click **Variables** and choose **Local 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_single_particle_variables.txt`.

SINGLE PARTICLE BATTERY (SPB)

Now start setting up the physics.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Single Particle Battery (spb)**.

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

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

4 Locate the **Battery Settings** section. In the ε_{pos} text field, type `epspos`.

5 In the ε_{neg} text field, type `epsneg`.

6 Locate the **Initial Charge Distribution** section. From the list, choose **Electrode state-of-charges**.

7 In the $SOC_{\mathrm{op,pos,0}}$ text field, type `opsocpos0`.

8 In the $SOC_{\mathrm{op,neg,0}}$ text field, type `opsocneg0`.

9 Locate the **Battery Volume** section. In the V_{cell} text field, type `Vcell`.

Electrolyte and Separator 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Single Particle Battery (spb)** click **Electrolyte and Separator 1**.

2 In the **Settings** window for **Electrolyte and Separator**, locate the **Electrolyte Settings** section.

3 In the c_{l} text field, type `cl`.

4 From the **Electrolyte solution resistance** list, choose **User defined**.

5 In the R_{sol} text field, type `Rsol`.

6 Locate the **Separator Settings** section. In the L_{sep} text field, type `Lsep`.

7 In the $\varepsilon_{\mathrm{sep}}$ text field, type `epssep`.

Positive Electrode 1

1 In the **Model Builder** window, click **Positive Electrode 1**.

2 In the **Settings** window for **Positive Electrode**, locate the **Electrode Settings** section.

3 In the ε_{s} text field, type `epsspos`.

4 Locate the **Material** section. From the **Particle material** list, choose **LMO, LiMn2O4 Spinel (Positive, Li-ion Battery) (mat1)**.

5 Locate the **Particle Transport Properties** section. From the D_{s} list, choose **User defined**. In the associated text field, type `Dspos`.

6 In the r_{p} text field, type `rppos`.

7 Click to expand the **Operational SOCs for Initial Cell Charge Distribution** section. From the $soc_{\min}$ list, choose **User defined**. In the associated text field, type `socminpos`.

8 From the $soc_{\max}$ list, choose **User defined**. In the associated text field, type `socmaxpos`.

9 Locate the **Model Input** section. In the T text field, type `T`.

Porous Electrode Reaction 1

1 In the **Model Builder** window, click **Porous Electrode Reaction 1**.

2 In the **Settings** window for **Porous Electrode Reaction**, locate the **Model Input** section.

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

4 Locate the **Material** section. From the **Material** list, choose **LMO, LiMn2O4 Spinel (Positive, Li-ion Battery) (mat1)**.

5 Locate the **Electrode Kinetics** section. From the **Exchange current density type** list, choose **Rate constant**.

6 In the k text field, type `kpos`.

7 In the $c_{\mathrm{l,ref}}$ text field, type `clref`.

Negative Electrode 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Single Particle Battery (spb)** click **Negative Electrode 1**.

2 In the **Settings** window for **Negative Electrode**, locate the **Electrode Settings** section.

3 In the ε_{s} text field, type `epssneg`.

4 Locate the **Species Settings** section. From the $c_{\mathrm{s,max}}$ list, choose **User defined**. In the associated text field, type `csmaxneg`.

5 Locate the **Particle Transport Properties** section. From the D_{s} list, choose **User defined**. In the associated text field, type `Dsneg`.

6 In the r_{p} text field, type `rpneg`.

7 Click to expand the **Operational SOCs for Initial Cell Charge Distribution** section. From the $soc_{\min}$ list, choose **User defined**. From the $soc_{\max}$ list, choose **User defined**. In the associated text field, type `socmaxneg`.

Porous Electrode Reaction 1

1 In the **Model Builder** window, click **Porous Electrode Reaction 1**.

2 In the **Settings** window for **Porous Electrode Reaction**, locate the **Model Input** section.

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

4 Locate the **Equilibrium Potential** section. From the E_{eq} list, choose **User defined**. In the associated text field, type `Eeqneg`.

5 Locate the **Electrode Kinetics** section. From the **Exchange current density type** list, choose **Rate constant**.

6 In the k text field, type `kneg`.

7 In the $c_{\mathrm{l,ref}}$ text field, type `clref`.

8 Click to expand the **Heat of Reaction** section. From the dE_{eq}/dT list, choose **User defined**.

STUDY 1

Perform a parametric study for different C-rates. Use Auxiliary Sweep in Study Extensions.

Step 2: Time Dependent

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

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

3 In the **Output times** text field, type `0 40000`.

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

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

6 Click to expand the **Study Extensions** section. Select the **Auxiliary sweep** check box.

7 Click + **Add**.

8 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
a (Multiplicative factor for the parametric study)	`0.1 1 2`	

Solution 1 (sol1)

1 In the **Study** toolbar, click **Show Default Solver**.

Store the actual steps taken by the solver to make sure to capture any sudden steep voltage changes.

2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node, then click **Time-Dependent Solver 1**.

3 In the **Settings** window for **Time-Dependent Solver**, locate the **General** section.

4 From the **Times to store** list, choose **Steps taken by solver**.

5 Right-click **Study 1>Solver Configurations>Solution 1 (sol1)>Time-Dependent Solver 1** and choose **Stop Condition**.

6 In the **Settings** window for **Stop Condition**, locate the **Stop Expressions** section.

7 Click + **Add**.

8 In the table, enter the following settings:

Stop expression	Stop if	Active	Description
`comp1.spb.E_cell<2.0`	True (>=1)	√	`Stop expression 1`

9 Locate the **Output at Stop** section. From the **Add solution** list, choose **Step before stop**.

10 Clear the **Add warning** check box.

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

RESULTS

Plot the discharge curves and compare them with text file data stemming from the original 1D model (Figure 1).

Cell Potential (spb)

1. In the **Model Builder** window, under **Results** click **Cell Potential (spb)**.
2. In the **Settings** window for **1D Plot Group**, click to expand the **Title** section.
3. From the **Title type** list, choose **Manual**.
4. In the **Title** text area, type `Discharge profiles`.
5. Locate the **Plot Settings** section. Select the **x-axis label** check box.
6. In the associated text field, type `Capacity (Ah/m<sup>2</sup>)`.
7. Select the **y-axis label** check box.
8. Locate the **Legend** section. From the **Position** list, choose **Lower left**.

Global

1. In the **Model Builder** window, expand the **Cell Potential (spb)** node, then click **Global**.
2. In the **Settings** window for **Global**, locate the **x-Axis Data** section.
3. From the **Parameter** list, choose **Expression**.
4. In the **Expression** text field, type `(t[s]/1[h])*i_1C*a`.
5. Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dash-dot**.
6. Click to expand the **Legends** section. From the **Legends** list, choose **Evaluated**.
7. In the **Legend** text field, type `Single particle model, eval(a) C`.
8. In the **Cell Potential (spb)** toolbar, click **Plot**.

Table 1

1. In the **Results** toolbar, click **Table**.
2. In the **Settings** window for **Table**, locate the **Data** section.
3. Click **Import**.
4. Browse to the model's Application Libraries folder and double-click the file `li_battery_single_particle_01C_comparison.txt`.

Table 2

1. In the **Results** toolbar, click **Table**.
2. In the **Settings** window for **Table**, locate the **Data** section.
3. Click **Import**.

4 Browse to the model's Application Libraries folder and double-click the file `li_battery_single_particle_1C_comparison.txt`.

Table 3

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

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

3 Click **Import**.

4 Browse to the model's Application Libraries folder and double-click the file `li_battery_single_particle_2C_comparison.txt`.

Table Graph 1

1 In the **Model Builder** window, right-click **Cell Potential (spb)** and choose **Table Graph**.

2 In the **Settings** window for **Table Graph**, locate the **Coloring and Style** section.

3 From the **Color** list, choose **Cycle (reset)**.

4 Find the **Line markers** subsection. From the **Marker** list, choose **Cycle**.

5 Click to expand the **Legends** section. Select the **Show legends** check box.

6 From the **Legends** list, choose **Manual**.

7 In the table, enter the following settings:

Legends
1D model, 0.1 C

Table Graph 2

1 Right-click **Table Graph 1** and choose **Duplicate**.

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

3 From the **Table** list, choose **Table 2**.

4 Locate the **Coloring and Style** section. From the **Color** list, choose **Cycle**.

5 Locate the **Legends** section. In the table, enter the following settings:

Legends
1D model, 1 C

Table Graph 3

1 Right-click **Table Graph 2** and choose **Duplicate**.

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

3 From the **Table** list, choose **Table 3**.

4 Locate the **Legends** section. In the table, enter the following settings:

Legends
1D model, 2 C

5 In the **Cell Potential (spb)** toolbar, click **Plot**.

SINGLE PARTICLE BATTERY (SPB)

Next, perform a charge discharge cycling study for a 1C rate.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Single Particle Battery (spb)**.

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

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

4 In the I_{dch} text field, type `Iapplied`.

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

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

7 In the $t_{\mathrm{rest,dch}}$ text field, type `trestdch`.

8 In the I_{ch} text field, type `-Iapplied`.

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

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

11 In the $t_{\mathrm{rest,ch}}$ text field, type `trestch`.

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 **Preset Studies for Selected Physics Interfaces>Time Dependent with Initialization**.

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

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

STUDY 2

Step 2: Time Dependent

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

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

3 In the **Output times** text field, type `range(0,10,8000)`.

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

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

Plot the charge discharge cycling potential and compare it with text file data stemming from the original 1D model (Figure 2).

Charge Discharge Cycling Potential

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

2 In the **Settings** window for **1D Plot Group**, type `Charge Discharge Cycling Potential` in the **Label** text field.

3 Locate the **Title** section. From the **Title type** list, choose **Label**.

4 Locate the **Plot Settings** section. Select the **x-axis label** check box.

5 In the associated text field, type `Time (s)`.

6 Select the **y-axis label** check box.

7 In the associated text field, type `Cell potential (V)`.

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

9 Locate the **Data** section. From the **Dataset** list, choose **Study 2/Solution 3 (sol3)**.

Global 1

1 Right-click **Charge Discharge Cycling Potential** 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)> Single Particle Battery>spb.E_cell - Cell potential - V**.

3 Locate the **Legends** section. From the **Legends** list, choose **Manual**.

4 In the table, enter the following settings:

Legends
`Single particle model`

Table 4

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

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

3 Click **Import**.

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

Table Graph 1

1 In the **Model Builder** window, right-click **Charge Discharge Cycling Potential** and choose **Table Graph**.

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

3 From the **Table** list, choose **Table 4**.

4 Locate the **Coloring and Style** section. Find the **Line markers** subsection. From the **Marker** list, choose **Circle**.

5 Locate the **Legends** section. Select the **Show legends** check box.

6 From the **Legends** list, choose **Manual**.

7 In the table, enter the following settings:

Legends
1D model

8 In the **Charge Discharge Cycling Potential** toolbar, click  **Plot**.