Created in COMSOL Multiphysics 6.2

Lithium-Ion Battery with Single-Ion Conducting Solid Electrolyte

Introduction

In solid-state lithium-ion batteries the electrolyte is a solid-state ionic conductor. The absence of a liquid electrolyte — and hence the lack of need for a liquid container and separator — implies a larger freedom of design. Additionally, solid electrolytes offer certain advantages such as no electrolyte leakage and improved thermal stability. The risk of the formation lithium metal dendrites, short-circuiting the battery cell, is also reduced when using a solid electrolyte.

Single-ion conducting electrolytes are typically synthesized by the immobilization of the counter-ion within an inorganic particle or a polymer backbone. These single-ion conductors have a transport number close to 1 and negligible concentration gradients with regards to the charge carrying ions.

This tutorial models a lithium-ion battery with a single-ion conducting solid electrolyte. The geometry is in one-dimension and the model is isothermal. The behavior at various discharge currents and solid electrolyte conductivities is analyzed. Additionally, a lithium-ion battery with a binary liquid electrolyte is simulated and its performance is compared to the solid state battery.

Model Definition

The model is set up for a graphite/LCO battery with a solid electrolyte. The electrode materials are available from the Battery Material Library and mainly default settings are selected. The conductivity of the solid electrolyte is set using a user-defined parameter.

The model is set up using the Lithium-Ion Battery, Single-Ion Conductor interface. This adds a Lithium-ion Battery interface with the charge balance model set to Single-Ion Conductor, that is typically applicable to solid electrolytes. In a single-ion conducting electrolyte it is assumed that only one ion is allowed to move, whereas the counter-ion is fixed. The assumption of electroneutrality and a constant concentration of the immobilized ions results in a constant concentration for the mobile lithium ions in the electrolyte. The Single-Ion Conductor charge balance model, thereby, solves for the electrolyte potential by assuming that all charge in the electrolyte phase is carried by the positive lithium ions only, so that the concentration of lithium ions in the electrolyte can be assumed to be constant. The electrolyte concentration is hence not solved for as a dependent variable.

The interface, with the single-ion conductor charge balance model, accounts for the following:

- charge transport in the electrode and electrolyte using Ohm's Law,
- material transport within the spherical particles that form the electrodes using Fick's Law, and
- Butler–Volmer electrode kinetics using experimentally measured discharge curves for the equilibrium potential.

This tutorial, as defined in the Modeling Instructions section below, consists of two parts. The first part simulates the discharge of a lithium-ion battery with a solid electrolyte, using the Single-Ion Conductor charge balance model, for a range of discharge currents and electrolyte conductivities. In the second part of the model, a lithium-ion battery with a binary liquid electrolyte is simulated and its performance is compared to that of the solid state battery for different discharge currents. Note that the model file available in Application Libraries contains the first part only.

The second part of the tutorial includes a binary liquid electrolyte, 1M $LiPF_6$ in 3:7 EC:EMC (available from the Battery Material Library). In this case, the Binary 1:1 Liquid Electrolyte charge balance model is used along with concentration dependent electrolyte conductivity. Note that the Binary 1:1 Liquid Electrolyte charge balance model additionally accounts for material transport in the electrolyte (that is, electrolyte concentration is solved for as a dependent variable), allowing for the introduction of the effects of concentration on ionic conductivity and concentration overpotential.

STUDY SETTINGS

The Time Dependent with Initialization study is used in this model. This study solves for a Current Distribution Initialization study step followed by a Time Dependent study step. A stop condition is used in the Time Dependent study step to stop the solver when the cell voltage reaches 2.7 V. The SOC and Initial Charge Distribution feature is used to define the initial charge inventory in the cell.

The study corresponding to the first part of the tutorial (solid electrolyte battery) sets up an Auxiliary sweep over discharge C-rates (1 C, 2 C, and 4 C) and solid electrolyte conductivities (0.02 S/m, 0.05 S/m, 0.5 S/m, and 1 S/m). The study corresponding to the second part of the tutorial (binary liquid electrolyte battery) sets up an Auxiliary sweep over discharge C-rates only.

Results and Discussion

Figure 1 and Figure 2 show the cell voltage profiles at electrolyte conductivity of 0.02 S/m and 1 S/m, respectively. The battery performance is higher at higher values of electrolyte conductivity. This is as expected, since the internal losses in the battery increase as the conductivity of the solid electrolyte is decreased.

Figure 1: Cell voltage profiles at electrolyte conductivity of 0.02 S/m.

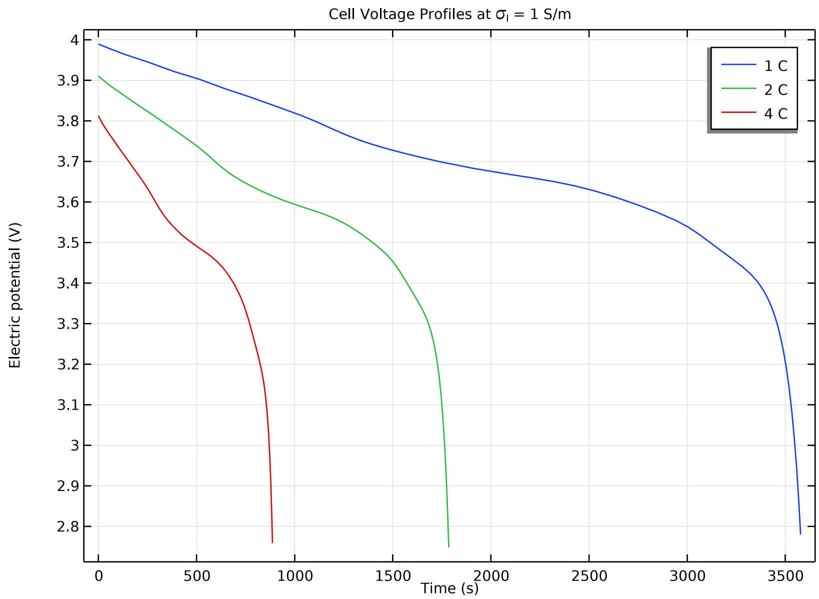

Figure 2: Cell voltage profiles at electrolyte conductivity of 1 S/m.

Figure 3 and Figure 4 show the 1 C discharge voltage profiles for different values of electrolyte conductivity ranging from 0.02 S/m to 1 S/m. The 4 C discharge profiles (Figure 4) clearly indicate decreased battery performance for lower values of electrolyte conductivity.

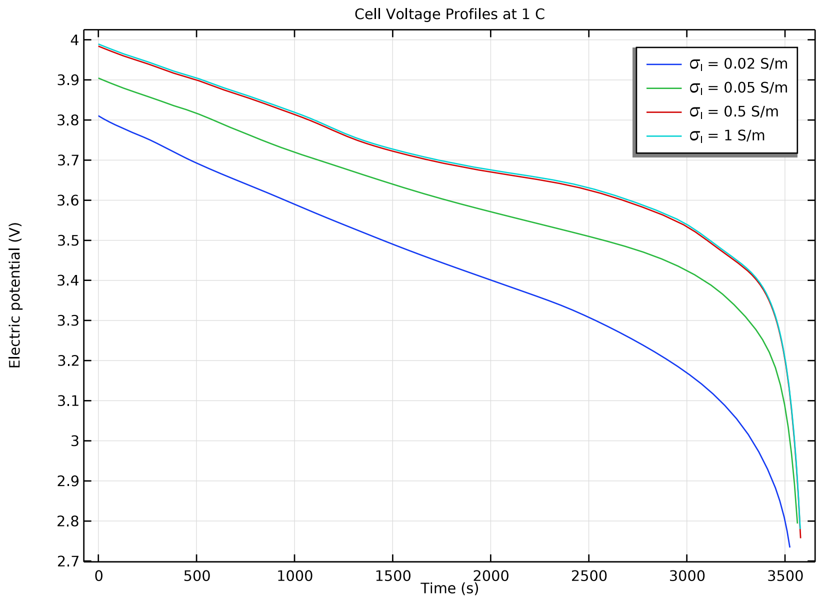

Figure 3: Cell voltage profiles at 1 C for different values of electrolyte conductivity.

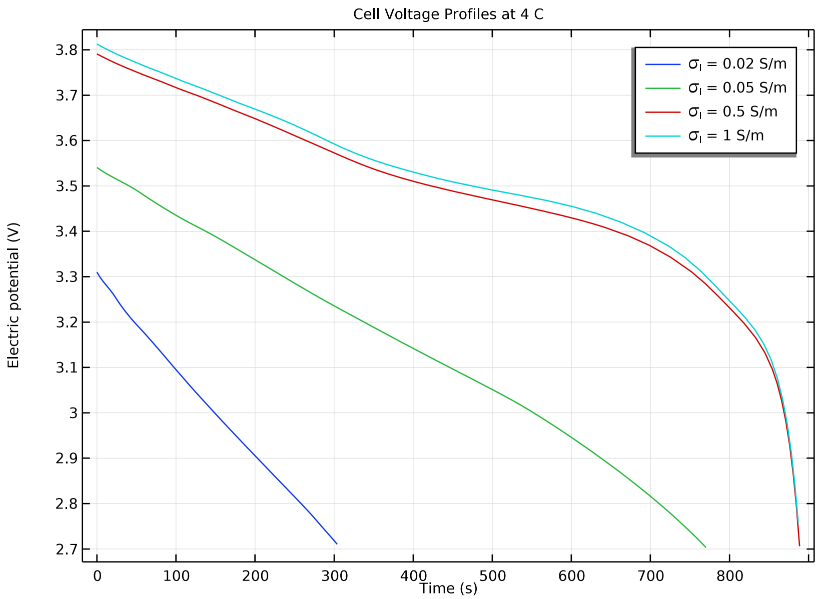

Figure 4: Cell voltage profiles at 4 C for different values of electrolyte conductivity.

Figure 5 and Figure 6 show the electrolyte potential drop across the cell at discharge rate of 1 C, for two different values of electrolyte conductivity. The voltage drop in the electrolyte is higher for lower values of electrolyte conductivity, as seen in Figure 5.

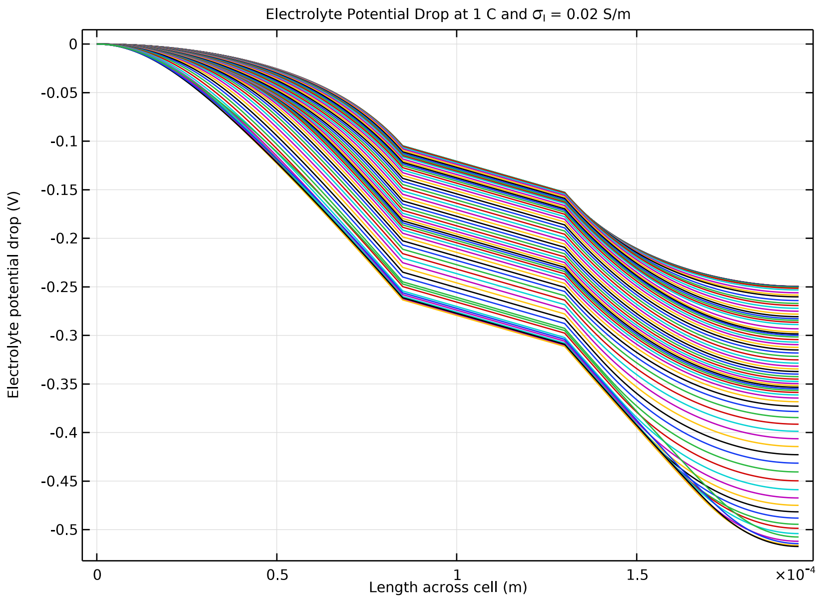

Figure 5: Electrolyte potential drop at 1 C and an electrolyte conductivity of 0.02 S/m.

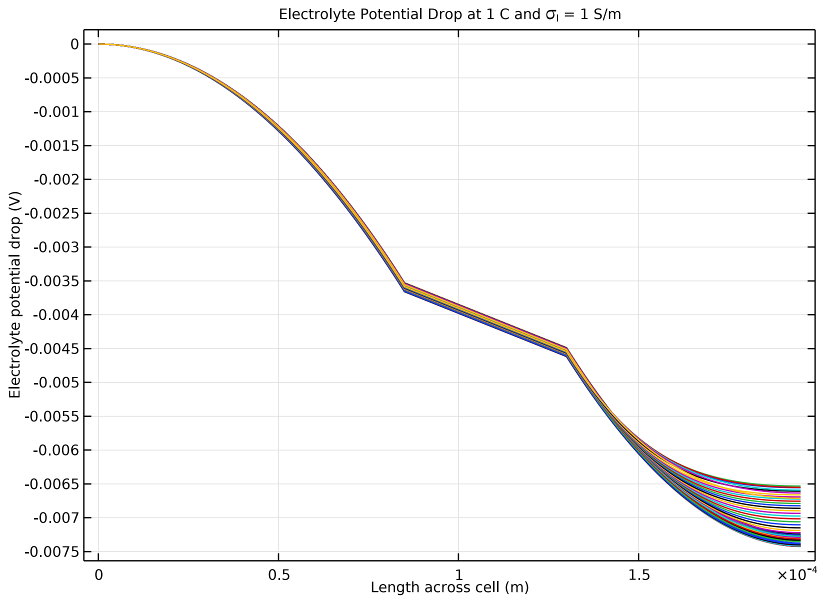

Figure 6: Electrolyte potential drop at 1 C and an electrolyte conductivity of 1 S/m.

Figure 7 shows a comparison of the cell voltage profiles for a battery with a solid electrolyte to that containing a binary liquid electrolyte. The electrolyte conductivity in the case of the solid electrolyte battery (modeled using the Single-Ion Conductor charge balance model) is considered to be 1 S/m. On the other hand, concentration dependent electrolyte conductivity is considered for the liquid electrolyte (1M $LiPF_6$ in 3:7 EC:EMC) used in the binary liquid electrolyte battery (modeled using the Binary 1:1 Liquid Electrolyte charge balance model). Since the conductivity of the binary liquid electrolyte at initial electrolyte concentration of 1M is nearly 1 S/m, the initial voltage at each discharge rate would be identical for both the solid and liquid electrolyte cases. The cell profiles would begin to differ at later discharge times, as the local conductivity for the binary liquid electrolyte battery begins to change due to concentration gradients. Additionally, the concentration gradients would be higher at higher discharge rates, indicating a greater difference at higher discharge rates, as seen in Figure 7.

The comparison plot also indicates that for a battery with a binary liquid electrolyte, one can use the Single-Ion Conductor charge balance model for simulating low discharge/charge scenarios where significant concentration gradients would not be expected. In such cases of low discharge/charge scenarios, the Single-Ion Conductor charge balance model would provide reduced computational loads, since the electrolyte concentration is not solved for as a degree of freedom, without significant loss in accuracy (particularly useful in the case of large models).

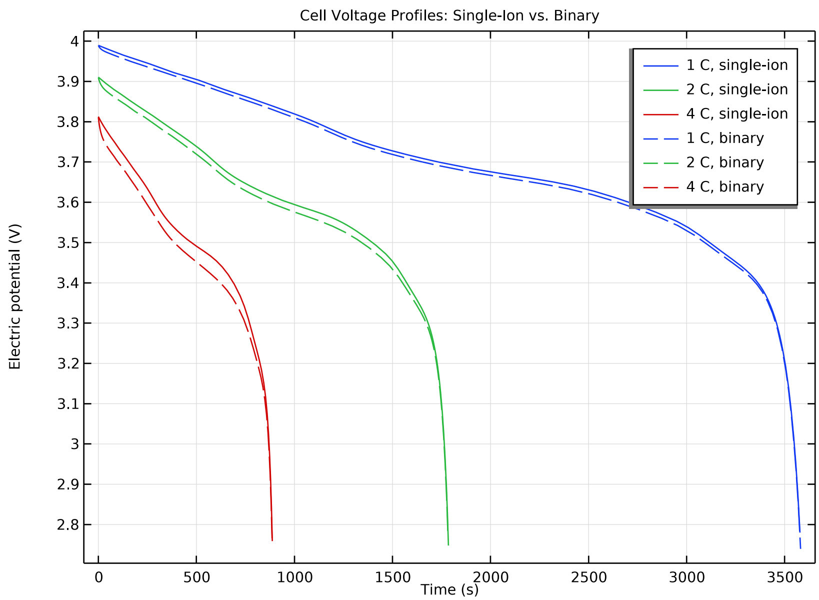

Figure 7: A comparison of the cell voltage profiles for the single-ion conductor (at electrolyte conductivity of 1 S/m) and binary liquid electrolyte charge balance models.

References

1. N. Wolff, F. Roder, and U. Krewer, "Model Based Assessment of Performance of Lithium-Ion Batteries Using Single-Ion Conducting Electrolytes," *Electrochimica Acta*, vol. 284, pp. 639–646, 2018.

2. S.D. Fabre, D. Guy-Bouyssou, P. Bouillon, F. Le Cras, and C. Delacourt, "Charge/Discharge Simulation of an All-Solid-State Thin-Film Battery Using a One-Dimensional Model," *J. Electrochemical Society*, vol. 159, pp. A104–A115, 2012.

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

Modeling Instructions

This tutorial consists of two parts. The first part simulates the discharge of a lithium-ion battery with a solid electrolyte, by using the Single-Ion Conductor charge balance model, for a range of discharge currents and electrolyte conductivities. The second part compares the performance of a lithium-ion battery containing a solid electrolyte to that containing a binary liquid electrolyte for different discharge currents. Note that the tutorial available in Application Libraries contains the first part only.

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

NEW

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

MODEL WIZARD

1 In the **Model Wizard** window, click **1D**.
2 In the **Select Physics** tree, select **Electrochemistry>Batteries>Lithium-Ion Battery, Single-Ion Conductor (liion)**.
3 Click **Add**.
4 Click **Study**.
5 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces> Time Dependent with Initialization**.

   (The **Time Dependent with Initialization study** will perform a time-dependent simulation, using an initialization study step to calculate the initial potentials in the cell.)
6 Click **Done**.

GLOBAL DEFINITIONS

Parameters 1

Load the parameters for this model 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 `li_battery_solid_electrolyte_parameters.txt`.

GEOMETRY 1

The geometry contains three domains. Create the geometry by specifying the lengths of the domains.

Interval 1 (i1)

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

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

3 From the **Specify** list, choose **Interval lengths**.

4 In the table, enter the following settings:

Lengths (m)
L_neg
L_electrolyte
L_pos

5 Click **Build Selected**.

ADD MATERIAL

The negative and positive electrode properties are specified using material properties (corresponding materials imported from the Battery Material Library), whereas the solid electrolyte properties are specified using user-defined parameters. The model has a graphite negative electrode and a LCO positive electrode.

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>Graphite, LixC6 MCMB (Negative, Li-ion Battery)**.

4 Click **Add to Component** in the window toolbar.

5 In the tree, select **Battery>Electrodes>LCO, LiCoO2 (Positive, Li-ion Battery)**.

6 Click **Add to Component** in the window toolbar.

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

MATERIALS

Graphite, LixC6 MCMB (Negative, Li-ion Battery) (mat1)

1 In the **Model Builder** window, under **Component 1 (comp1)>Materials** click **Graphite, LixC6 MCMB (Negative, Li-ion Battery) (mat1)**.

2 In the **Settings** window for **Material**, locate the **Geometric Entity Selection** section.

3 Click **Clear Selection**.

4 Select Domain 1 only.

LCO, LiCoO2 (Positive, Li-ion Battery) (mat2)

1 In the **Model Builder** window, click **LCO, LiCoO2 (Positive, Li-ion Battery) (mat2)**.

2 Select Domain 3 only.

DEFINITIONS

Load the variables for this model 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_solid_electrolyte_variables.txt`.

Integration 1 (intop1)

Define boundary integration variables in order to access the cell voltage at the end terminals during computation and postprocessing.

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

2 In the **Settings** window for **Integration**, type `PositiveCC` in the **Operator name** text field.

3 Locate the **Source Selection** section. From the **Geometric entity level** list, choose **Boundary**.

4 Select Boundary 4 only.

Integration 1 (PositiveCC)

Right-click **Integration 1 (PositiveCC)** and choose **Duplicate**.

Integration 2 (PositiveCC2)

1 In the **Model Builder** window, under **Component 1 (comp1)>Definitions** click **Integration 2 (PositiveCC2)**.

2 In the **Settings** window for **Integration**, type `NegativeCC` in the **Operator name** text field.

3 Locate the **Source Selection** section. Click **Clear Selection**.

4 Select Boundary 1 only.

LITHIUM-ION BATTERY (LIION)

Set up the physics in the model. Use the **SOC and Initial Charge Distribution** node in order to calculate the initial charge distribution in the cell.

Separator 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Lithium-Ion Battery (liion)** click **Separator 1**.

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

3 From the σ_l list, choose **User defined**. In the associated text field, type `sigmal`.

Porous Electrode 1

1 In the **Physics** toolbar, click **Domains** and choose **Porous Electrode**.

2 Select Domain 1 only.

3 In the **Settings** window for **Porous Electrode**, locate the **Electrolyte Properties** section.

4 From the σ_l list, choose **User defined**. In the associated text field, type `sigmal`.

5 Locate the **Electrode Properties** section. In the σ_s text field, type `sigmas_neg`.

6 Locate the **Porous Matrix Properties** section. In the ε_s text field, type `epss_neg`.

Particle Intercalation 1

1 In the **Model Builder** window, click **Particle Intercalation 1**.

2 In the **Settings** window for **Particle Intercalation**, locate the **Particle Transport Properties** section.

3 In the r_p text field, type `rp`.

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 **Electrode Kinetics** section.

3 In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0ref_neg`.

Porous Electrode 2

1 In the **Physics** toolbar, click **Domains** and choose **Porous Electrode**.

2 Select Domain 3 only.

3 In the **Settings** window for **Porous Electrode**, locate the **Electrolyte Properties** section.

4 From the σ_l list, choose **User defined**. In the associated text field, type `sigmal`.

5 Locate the **Electrode Properties** section. In the σ_s text field, type `sigmas_pos`.

6 Locate the **Porous Matrix Properties** section. In the ε_s text field, type `epss_pos`.

Particle Intercalation 1

1. In the **Model Builder** window, click **Particle Intercalation 1**.
2. In the **Settings** window for **Particle Intercalation**, locate the **Particle Transport Properties** section.
3. In the r_p text field, type `rp`.

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 **Electrode Kinetics** section.
3. In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0ref_pos`.
4. In the **Model Builder** window, click **Lithium-Ion Battery (liion)**.
5. In the **Settings** window for **Lithium-Ion Battery**, locate the **Cell Settings** section.
6. Select the **Define cell state of charge (SOC) and initial charge inventory** check box.

SOC and Initial Charge Distribution 1

1. In the **Model Builder** window, under **Component 1 (comp1)>Lithium-Ion Battery (liion)** click **SOC and Initial Charge Distribution 1**.
2. In the **Settings** window for **SOC and Initial Charge Distribution**, locate the **Initial Cell Charge Distribution** section.
3. In the SOC_0 text field, type `SOC_0`.
4. Clear the **Add formation loss** check box.

Negative Electrode Selection 1

Select which model domains that represent the negative and positive electrode, respectively.

1. In the **Model Builder** window, click **Negative Electrode Selection 1**.
2. Select Domain 1 only.

Positive Electrode Selection 1

1. In the **Model Builder** window, click **Positive Electrode Selection 1**.
2. Select Domain 3 only.

Electric Ground 1

Finish by setting the boundary conditions. Ground is set as reference at the leftmost boundary, the negative electrode current collector. A current is applied at the rightmost boundary, the positive electrode current collector. Note that 1C current is available from the **SOC and Initial Charge Distribution** node.

1 In the **Physics** toolbar, click **Boundaries** and choose **Electric Ground**.
2 Select Boundary 1 only.

Electrode Current 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Electrode Current**.
2 Select Boundary 4 only.
3 In the **Settings** window for **Electrode Current**, locate the **Electrode Current** section.
4 In the $I_{s,total}$ text field, type `-I_app`.
5 In the $\phi_{s,bnd,init}$ text field, type `4[V]`.

STUDY 1

Modify the **Time Dependent with Initialization study**, to perform an Auxiliary sweep over discharge C-rates and solid electrolyte conductivities.

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 4000`.
4 Click to expand the **Study Extensions** section. Select the **Auxiliary sweep** check box.
5 From the **Sweep type** list, choose **All combinations**.
6 Click **Add**.
7 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
C_rate (C-rate parameter)	1 2 4	

8 Click **Add**.
9 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
sigmal (Electrolyte conductivity)	0.02 0.05 0.5 1	S/m

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.PositiveCC(comp1.phis) <2.7`	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 **Model Builder** window, click **Study 1**.

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

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

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

RESULTS

Reproduce the plots in the model documentation, starting with the cell voltage profiles at electrolyte conductivity of 0.02S/m (Figure 1).

Cell Voltage: sigmal = 0.02 S/m

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

2 In the **Settings** window for **1D Plot Group**, type `Cell Voltage: sigmal = 0.02 S/m` in the **Label** text field.

3 Locate the **Data** section. From the **Parameter selection (sigmal)** list, choose **First**.

Point Graph 1

1 Right-click **Cell Voltage: sigmal = 0.02 S/m** and choose **Point Graph**.

2 Select Boundary 4 only.

3 In the **Settings** window for **Point Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Lithium-Ion Battery>phis - Electric potential - V**.

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

5 From the **Legends** list, choose **Evaluated**.

6 In the **Legend** text field, type eval(C_rate) C.

Cell Voltage: sigmal = 0.02 S/m

1 In the **Model Builder** window, click **Cell Voltage: sigmal = 0.02 S/m**.

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 Cell Voltage Profiles at \sigma_l = 0.02 S/m.

5 In the **Cell Voltage: sigmal = 0.02 S/m** toolbar, click **Plot**.

Now, duplicate the previous figure to create a plot of the cell voltage profiles at electrolyte conductivity of 1S/m (Figure 2).

Right-click **Cell Voltage: sigmal = 0.02 S/m** and choose **Duplicate**.

Cell Voltage: sigmal = 1 S/m

1 In the **Model Builder** window, under **Results** click **Cell Voltage: sigmal = 0.02 S/m 1**.

2 In the **Settings** window for **1D Plot Group**, type Cell Voltage: sigmal = 1 S/m in the **Label** text field.

3 Locate the **Data** section. From the **Parameter selection (sigmal)** list, choose **Last**.

4 Locate the **Title** section. In the **Title** text area, type Cell Voltage Profiles at \sigma_l = 1 S/m.

5 In the **Cell Voltage: sigmal = 1 S/m** toolbar, click **Plot**.

Cell Voltage: 1 C

Next, create cell voltage profiles plots at 1 C (Figure 3) and 4 C (Figure 4), respectively, for different value of electrolyte conductivity.

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

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

3 Locate the **Data** section. From the **Parameter selection (C_rate)** list, choose **First**.

Point Graph 1

1. Right-click **Cell Voltage: 1 C** and choose **Point Graph**.
2. Select Boundary 4 only.
3. In the **Settings** window for **Point Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)> Lithium-Ion Battery>phis - Electric potential - V**.
4. Locate the **Legends** section. Select the **Show legends** check box.
5. From the **Legends** list, choose **Evaluated**.
6. In the **Legend** text field, type \sigma_l = eval(sigmal) S/m.

Cell Voltage: 1 C

1. In the **Model Builder** window, click **Cell Voltage: 1 C**.
2. In the **Settings** window for **1D Plot Group**, locate the **Title** section.
3. From the **Title type** list, choose **Manual**.
4. In the **Title** text area, type Cell Voltage Profiles at 1 C.
5. In the **Cell Voltage: 1 C** toolbar, click **Plot**.
6. Right-click **Cell Voltage: 1 C** and choose **Duplicate**.

Cell Voltage: 4 C

1. In the **Model Builder** window, under **Results** click **Cell Voltage: 1 C 1**.
2. In the **Settings** window for **1D Plot Group**, type Cell Voltage: 4 C in the **Label** text field.
3. Locate the **Data** section. From the **Parameter selection (C_rate)** list, choose **Last**.
4. Locate the **Title** section. In the **Title** text area, type Cell Voltage Profiles at 4 C.
5. In the **Cell Voltage: 4 C** toolbar, click **Plot**.

Electrolyte Potential Drop: 1 C and sigmal = 0.02 S/m

Next, create plots depicting the electrolyte potential drop at 1C, for two values of electrolyte conductivity. Figure 5 and Figure 6 correspond, respectively, to electrolyte conductivity values of 0.02S/m and 1S/m.

1. In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.
2. In the **Settings** window for **1D Plot Group**, type Electrolyte Potential Drop: 1 C and sigmal = 0.02 S/m in the **Label** text field.
3. Locate the **Data** section. From the **Parameter selection (C_rate)** list, choose **First**.
4. From the **Parameter selection (sigmal)** list, choose **First**.

Line Graph 1

1. Right-click **Electrolyte Potential Drop: 1 C and sigmal = 0.02 S/m** and choose **Line Graph**.
2. In the **Settings** window for **Line Graph**, locate the **Selection** section.
3. From the **Selection** list, choose **All domains**.
4. Locate the **y-Axis Data** section. In the **Expression** text field, type phil-NegativeCC(phil).

Electrolyte Potential Drop: 1 C and sigmal = 0.02 S/m

1. In the **Model Builder** window, click **Electrolyte Potential Drop: 1 C and sigmal = 0.02 S/m**.
2. In the **Settings** window for **1D Plot Group**, locate the **Title** section.
3. From the **Title type** list, choose **Manual**.
4. In the **Title** text area, type Electrolyte Potential Drop at 1 C and \sigma_l = 0.02 S/m.
5. Locate the **Plot Settings** section.
6. Select the **x-axis label** check box. In the associated text field, type Length across cell (m).
7. Select the **y-axis label** check box. In the associated text field, type Electrolyte potential drop (V).
8. In the **Electrolyte Potential Drop: 1 C and sigmal = 0.02 S/m** toolbar, click **Plot**.
9. Right-click **Electrolyte Potential Drop: 1 C and sigmal = 0.02 S/m** and choose **Duplicate**.

Electrolyte Potential Drop: 1 C and sigmal = 1 S/m

1. In the **Model Builder** window, under **Results** click **Electrolyte Potential Drop: 1 C and sigmal = 0.02 S/m 1**.
2. In the **Settings** window for **1D Plot Group**, type Electrolyte Potential Drop: 1 C and sigmal = 1 S/m in the **Label** text field.
3. Locate the **Data** section. From the **Parameter selection (sigmal)** list, choose **Last**.
4. Locate the **Title** section. In the **Title** text area, type Electrolyte Potential Drop at 1 C and \sigma_l = 1 S/m.
5. In the **Electrolyte Potential Drop: 1 C and sigmal = 1 S/m** toolbar, click **Plot**.

MATERIALS

The first part of the tutorial is now complete. In the second part, the performance of a lithium-ion battery containing a solid electrolyte is compared to that containing a binary liquid electrolyte. Now let us proceed to modify the model setup for a binary liquid electrolyte. Start by adding an electrolyte material and subsequently modifying the physics settings.

ADD MATERIAL

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>Electrolytes>LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery)**.

4 Click **Add to Component** in the window toolbar.

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

MATERIALS

LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery) (mat3)

Select Domain 2 only.

LITHIUM-ION BATTERY (LIION)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Lithium-Ion Battery (liion)**.

2 In the **Settings** window for **Lithium-Ion Battery**, locate the **Charge Balance Model** section.

3 From the list, choose **Binary 1:1 liquid electrolyte**.

Separator 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Lithium-Ion Battery (liion)** click **Separator 1**.

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

3 From the σ_l list, choose **From material**.

Porous Electrode 1

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

2 In the **Settings** window for **Porous Electrode**, locate the **Electrolyte Properties** section.

3 From the **Electrolyte material** list, choose **LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery) (mat3)**.

4 From the σ_l list, choose **From material**.

Porous Electrode 2

1 In the **Model Builder** window, click **Porous Electrode 2**.

2 In the **Settings** window for **Porous Electrode**, locate the **Electrolyte Properties** section.

3 From the **Electrolyte material** list, choose **LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery) (mat3)**.

4 From the σ_l list, choose **From material**.

ADD STUDY

Add a **Time Dependent with Initialization study** as before, to perform an Auxiliary sweep over discharge C-rates.

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 `0 4000`.

4 Locate the **Study Extensions** section. Select the **Auxiliary sweep** check box.

5 Click **Add**.

6 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
C_rate (C-rate parameter)	1 2 4	

Solution 3 (sol3)

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

2 In the **Model Builder** window, expand the **Solution 3 (sol3)** 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 In the **Model Builder** window, expand the **Study 2>Solver Configurations> Solution 3 (sol3)>Time-Dependent Solver 1** node.

6 Right-click **Study 2>Solver Configurations>Solution 3 (sol3)>Time-Dependent Solver 1** and choose **Stop Condition**.

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

8 Click **Add**.

9 In the table, enter the following settings:

Stop expression	Stop if	Active	Description
`comp1.PositiveCC(comp1.phis) <2.7`	True (>=1)	√	`Stop expression 1`

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

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

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

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

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

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

RESULTS

Cell Voltage: Single-Ion vs. Binary

Finally, create a plot that compares the cell voltage profiles for the single-ion conductor (at electrolyte conductivity of 1S/m) and binary liquid electrolyte charge balance models (Figure 7).

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

2 In the **Settings** window for **1D Plot Group**, type `Cell Voltage: Single-Ion vs. Binary` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **None**.

Point Graph 1

1 Right-click **Cell Voltage: Single-Ion vs. Binary** and choose **Point Graph**.

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

3 From the **Dataset** list, choose **Study 1/Solution 1 (sol1)**.

4 From the **Parameter selection (sigmal)** list, choose **Last**.

5 Select Boundary 4 only.

6 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Lithium-Ion Battery>phis - Electric potential - V**.

7 Locate the **x-Axis Data** section. From the **Axis source data** list, choose **Time**.

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

9 From the **Legends** list, choose **Evaluated**.

10 In the **Legend** text field, type `eval(C_rate) C, single-ion`.

11 Right-click **Point Graph 1** and choose **Duplicate**.

Point Graph 2

1 In the **Model Builder** window, click **Point Graph 2**.

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

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

4 Click to expand 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. In the **Legend** text field, type `eval(C_rate) C, binary`.

Cell Voltage: Single-Ion vs. Binary

1 In the **Model Builder** window, click **Cell Voltage: Single-Ion vs. Binary**.

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

3 From the **Title type** list, choose **Manual**.

4 In the **Title** text area, type `Cell Voltage Profiles: Single-Ion vs. Binary`.

5 In the **Cell Voltage: Single-Ion vs. Binary** toolbar, click **Plot**.