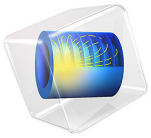

Model created in COMSOL Multiphysics 6.4

LMO Decomposition

Introduction

Some positive electrode materials are known to deteriorate in overcharged lithium-ion battery cells. Predominantly, manganese-containing electrode materials such as LMO and NMC can lose capacity due to manganese dissolution when overcharged. This decomposition is a chemical reaction driven by protons that originate from solvent oxidation and water. The reaction decreases the electrode volume fraction.

This example models the capacity fade of an LMO vs. Li(s) cell. An abusive cycling condition, with repeated C/3 charge-discharge cycling between 3.6 V and 4.5 V at elevated temperature, is investigated.

Model Definition

GENERAL

The model is set up in 1D for a Li(s)/LMO cell with a 1.0 M $LiPF_6$ in EC:EMC (3:7 by weight) electrolyte. The lithium foil is defined at a boundary and the LMO porous electrode at a domain. The two electrodes are parted by a separator (Figure 1).

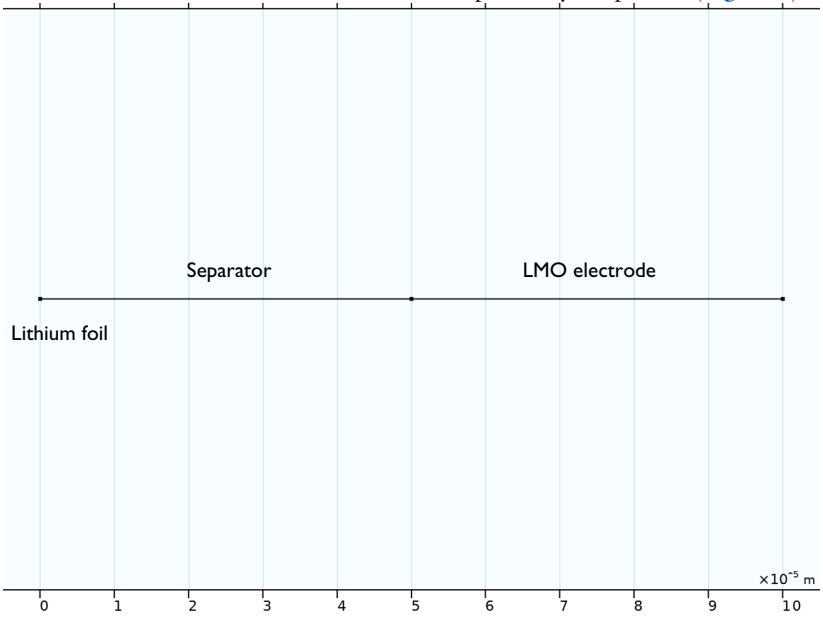

Figure 1: Model geometry.

The Lithium-Ion Battery interface is used, accounting for:

- Electronic conduction in the LMO electrode
- Ionic charge transport in the electrode and electrolyte/separator
- Material transport in the electrolyte, allowing for including the effects of concentration on ionic conductivity and concentration overpotentials
- Material transport within solid spherical particles in the LMO electrode
- Butler–Volmer electrode intercalation kinetics using experimentally measured equilibrium potentials
- Electrode surface with Butler–Volmer kinetics for lithium foil

Most material properties are taken from the Battery material library. More information about how to use the Lithium-Ion Battery interface can be found in the 1D Isothermal Lithium-Ion Battery example.

Additional features are used in the Lithium-Ion Battery interface to account for the detrimental electrochemical and chemical reactions. The Transport of Diluted Species interface is used to define the reactions and transport of foreign species in the cell.

DETRIMENTAL REACTIONS

Several reactions are involved in the LMO decomposition and are accounted for in the model. In short, solvent oxidation is the triggering reaction as the presence of protons in the electrolyte maintains the decomposition. The detrimental reaction details are described below (Ref. 1).

Solvent Oxidation

At 4.2 V cell voltage, the solvent is electrochemically decomposed at the electronically conductive material of the LMO electrode:

$$\text{Solvent} \rightarrow \text{Solvent}^{*} + \text{H}^{+} + \text{e}^{-}$$

The reaction is assumed to be irreversible and the loss of solvent is neglected, that is, exhausted and fresh solvent is assumed to behave in the same manner. Anodic Tafel kinetics are set, giving the following volumetric reaction source, $r_{\text{v,oxid}}$ (mol/(m^3·s)):

$$r_{\text{v, oxid}} = \frac{-a_{\text{cs}}\nu_{\text{H}} i_{0,\text{ oxid}}}{F}\left(\frac{c_{\text{l}}}{c_{\text{l, ref}}}\right)^{0.5} \exp\left(\frac{F}{2RT}(\phi_{\text{s}} - \phi_{\text{l,ps}} - E_{\text{eq, oxid}})\right) \quad (1)$$

LMO Decomposition by Protons

Manganese dissolves as LMO ($LiMn_2O_4$) decomposes in an irreversible chemical reaction driven by protons:

$$4H^+ + 2LiMn_2O_4 \rightarrow 2Li^+ + Mn^{2+} + \frac{3}{2}LiMn_2O_4 + 2H_2O$$

The volumetric reaction source, $r_{v,proton}$, is defined as:

$$r_{v,\,proton} = a_S k_{proton} c_H \tag{2}$$

Electrolyte Salt Loss by Water

Electrolyte salt decomposes irreversibly with water. The model assumes that one Li^+ is lost as LiF and that HF is fully ionized:

$$LiPF_6 + H_2O \rightarrow LiF + POF_3 + 2H^+ + 2F^-$$

The volumetric reaction source, $r_{v,water}$, depends on the water and electrolyte salt concentrations:

$$r_{v,\,water} = k_{water} c_{H_2O}^2 c_l \tag{3}$$

Additional Electrochemical Reactions at Lithium Foil

The concentrations of protons and manganese ions in the electrolyte are counteracted by reduction reactions at the lithium foil surface. For simplicity, only reductions are considered and the products are said to be inert:

$$2H^+ + 2e^- \rightarrow H_2$$

$$Mn^{2+} + 2e^- \rightarrow Mn(s)$$

The reduction reactions are defined using cathodic Tafel kinetics, giving the following reaction rate fluxes, N_i (mol/(m^2·s)):

$$N_H = \frac{-\nu_H i_{0,\,H,\,ref}}{F} \frac{c_H}{c_{H,\,ref}} \exp\left(-\frac{F}{2RT}(\phi_s - \phi_{l,ps} - E_{eq,\,H,\,ref})\right) \tag{4}$$

$$N_{Mn} = \frac{-\nu_{Mn} i_{0,\,Mn,\,ref}}{2F} \frac{c_{Mn}}{c_{Mn,\,ref}} \exp\left(-\frac{F}{2RT}(\phi_s - \phi_{l,ps} - E_{eq,\,Mn,\,ref})\right) \tag{5}$$

In the expressions in the sections above:

- a_{cs} is the specific surface area at the electronically conductive material set to 10^6 m^{-1}.
- a_s, is the specific surface area of the electrode material defined by the electrode material volume fraction, ε_s, and the radius of the LMO particles, r_{LMO}:

$$a_s = \frac{3\varepsilon_s}{r_{LMO}} \tag{6}$$

- c_i is the concentration of species i.
- $c_{i,ref}$ is the reference concentration of i.
- $i_{0,\,oxid}$ is the exchange current density of the solvent oxidation.
- $i_{0,\,i,\,ref}$ is the exchange current density of i at the reference concentration.
- k_{proton} (m/s) is the rate constant of the LMO decomposition by protons reaction.
- k_{water} (m^6/(mol·s)) is the rate constant for the electrolyte salt loss by water reaction.
- $E_{eq,\,oxid}$ is the equilibrium potential of the solvent oxidation.
- $E_{eq,\,i,\,ref}$ is the reference equilibrium potential of the reduction of i.
- ν_i is the stoichiometric coefficient of i in the electrochemical reaction.
- The electrochemical reactions are dependent on the solid phase potential, ϕ_s, and the pseudo-potentiostatic electrolyte potential, $\phi_{l,ps}$. The latter is used instead of the electrolyte phase potential variable, ϕ_l, and includes an ideal electrolyte concentration dependence for single charged ions (that is, the dominating charge of ions in this example). For more information, see the Copper Current-Collector Dissolution example.

DETRIMENTAL REACTIONS IN THE LITHIUM-ION BATTERY INTERFACE

Foreign Species

Since the Lithium-Ion Battery interface is primarily intended for a binary electrolyte (Li^+/PF_6^- with solvent), the addition of foreign species requires some assumptions to be made. In this example, all cations are treated as Li^+ and any unreacted water is considered to constitute a negligible part of the solvent. This approach means that electroneutrality can be ensured at all times and that the salt transport is affected by the total concentration of species in the electrolyte.

Electrochemical Reactions

At the LMO, the solvent oxidation reaction is defined as an additional reaction to the main lithium intercalation reaction. This is done using an additional **Porous Electrode Reaction** in the **Porous Electrode** node.

At the lithium foil boundary, the proton and manganese ion reductions are defined as additional reactions to the lithium reaction. This is done by adding an **Electrode Reaction** subnode for each reduction in the **Electrode Surface** node.

The reactions give a net change of cations. The stoichiometric coefficients for each cation, ν_i, will be represented by the stoichiometric coefficient of Li^+, ν_{Li+}, (Equation 1-Equation 5) following the assumption above. Therefore, for the proton reduction and solvent oxidation reactions, the coefficient will be set to –1 and for the manganese deposition –2 (two Li^+ for each Mn^{2+}).

Chemical Reactions

The net change of cations from the chemical reactions need to be accounted for as well. The LMO decomposition gives no net change in cations. However, the electrolyte salt loss gives a net increase of ions, as two H^+ and two F^- are formed on the expense of one Li^+ and one LF_6^-. Assuming that both anions behave in a similar way, the cation volumetric reaction source, $r_{v,\,cation}$, is defined as:

$$r_{v,\,cation} = r_{v,\,water} \tag{7}$$

The cation source is defined using a **Reaction Source** node that can be added when the **Advanced Physics Options** is enabled.

Loss of Electrode Volume Fraction

The LMO decomposition results in a loss in electrode (LMO) volume fraction, ε_s. The **Dissolving–Depositing Species** section of the **Porous Electrode** node is used to solve for an additional degree of freedom to keep track of the concentration of exhausted LMO, $c_{LMOdead}$ (mol/m^3), according to:

$$\frac{dc_{LMO_{dead}}}{dt} = -r_{v,\,proton} \tag{8}$$

The reaction rate is defined using a **Nonfaraidaic Reactions** subnode. With the **Add volume change to electrode volume fraction** enabled in the **Porous Electrode** node, the change in electrode volume fraction, $\Delta\varepsilon_s$, is computed with the molar volume of LMO, V_m, as follows:

$$\Delta\varepsilon_s = c_{LMO_{dead}} V_m \tag{9}$$

Furthermore, the electrolyte volume fraction is set as constant in the model, assuming that the molar volume of LMO is unchanged.

Inhibited Transport in LMO Material

Lithium transport in the remaining LMO material is, in accordance with Ref. 1, inhibited from forming an inactive film consisting of precipitated decomposition products. This example incorporates the relationship between the diffusion coefficient, D_{LMO}, and the electrode volume fraction, given by:

$$D_{\mathrm{LMO}} = D_{\mathrm{LMO},0}\left(1-\left(\frac{\varepsilon_{\mathrm{s},0}-\varepsilon_{\mathrm{s}}}{\varepsilon_{\mathrm{s},0}}\right)^{n_n}\right) \tag{10}$$

In the equation, the subscript 0 indicates the state at the beginning of cycling and n_{s} is an adjust factor typically fitted to experimental results.

DETRIMENTAL REACTIONS IN THE TRANSPORT OF DILUTED SPECIES INTERFACE

The foreign species concentrations are assumed to be low in comparison to the Li^+/PF_6^- (+ solvent) electrolyte, and therefore a dilute approximation of the transport and electrochemical reactions is valid. It follows that the electrolyte phase potential field is governed by the lithium-ion transport, and that the contribution to the electrolyte potential field from the foreign species transport may be neglected.

The Transport of Diluted Species interface solves for the transport of foreign species by diffusion and migration. For the migration term, the pseudopotentiostatic electrolyte potential, $\phi_{\mathrm{l\,ps}}$, is used. On the lithium foil boundary, the fluxes due to proton reduction and manganese deposition are computed using the **Electrode Surface Coupling** node. At the LMO porous electrode, the **Porous Electrode Coupling** node is used to account for the solvent oxidation reaction. All chemical reactions are defined using **Reactions** nodes.

ELECTROLYTE SALT CONCENTRATION

In accordance to the definitions and assumptions above, the $LiPF_6$ concentration, $c_{\mathrm{l,net}}$, is given by the difference in electrolyte salt concentration, c_{l}, as computed by the Lithium-Ion Battery interface (in other words the total concentration of cations) and the foreign cation concentrations:

$$c_{\mathrm{l,net}} = c_{\mathrm{l}} - c_{\mathrm{H}} - 2c_{\mathrm{Mn}} \tag{11}$$

The difference between the first and last C/3 discharge cycle can be seen in Figure 2. Results indicate considerable capacity fade.

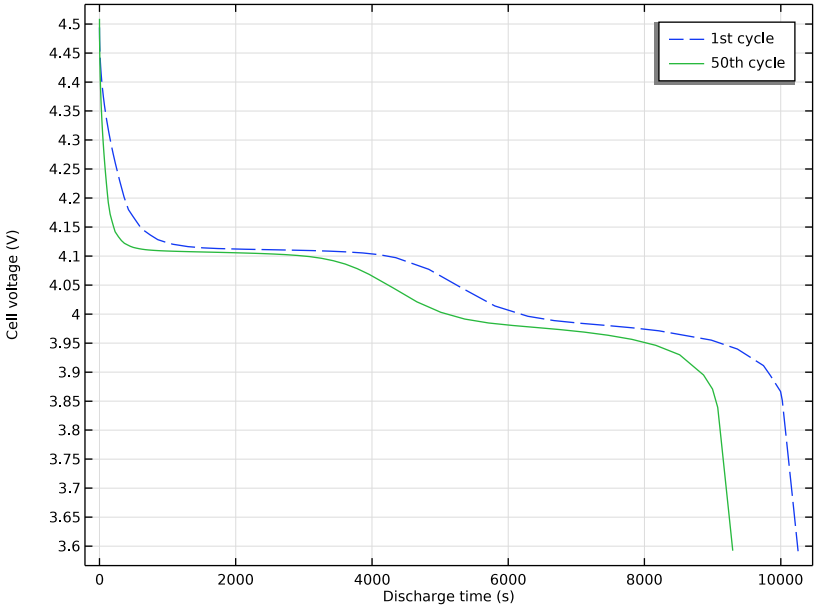

Figure 2: 1st and 50th discharge curves taken from continuous C/3 charge-discharge cycling of the LMO versus Li(s) cell at 328 K.

In Figure 3, the loss in electrode (LMO) volume fraction in the porous electrode after 50 cycles is shown to be about 4%.

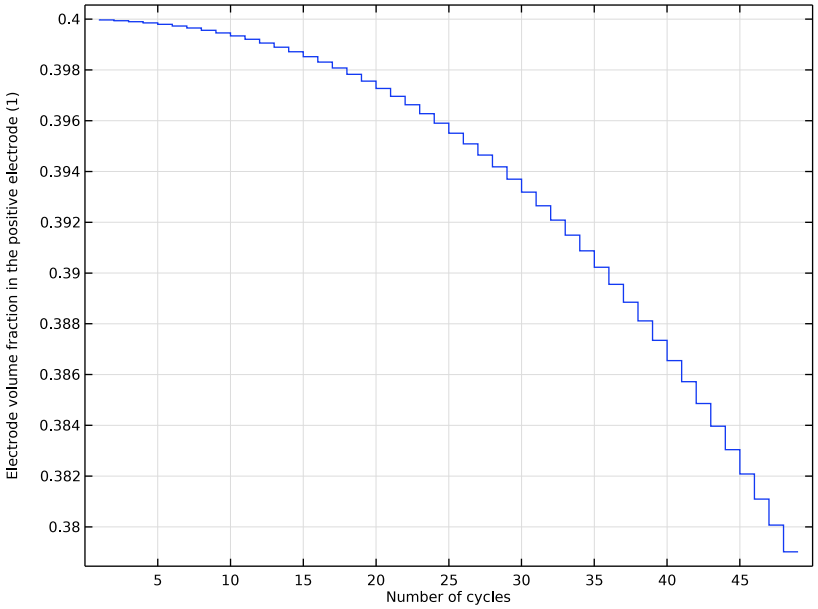

Figure 3: Electrode volume fraction in the porous electrode with cycling.

Figure 4 displays the decrease in the diffusion coefficient of lithium within the LMO particles with cycling. The decrease declines with the number of cycles.

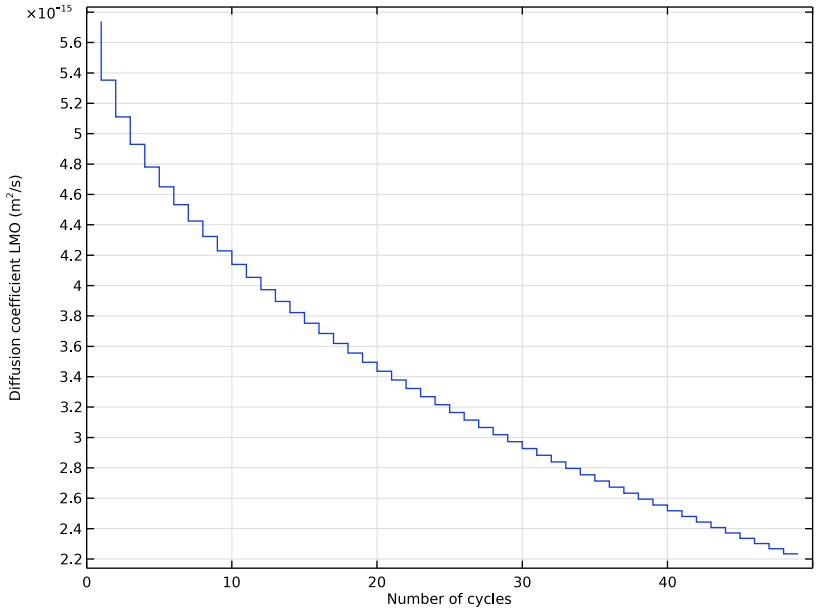

Figure 4: Diffusion coefficient of lithium within the LMO particles with cycling.

The relative capacity of the cell decreases over time as shown in Figure 5. The capacity based on cyclable lithium and host capacity follows the electrode volume fraction. The nominal C/3 discharge capacity declines more with time since this capacity captures the increased polarization caused by the lowered diffusion coefficient of lithium in LMO.

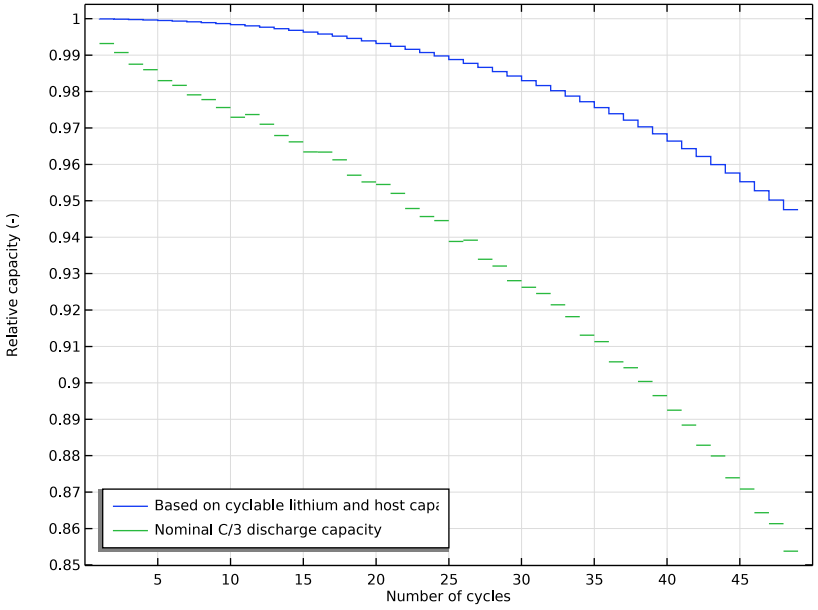

Figure 5: Change in relative capacity with cycling.

In Figure 6, the change in electrolyte salt concentration shows the LMO decomposition reaction to be dominant after about 12 cycles increasing the salt concentration considerably.

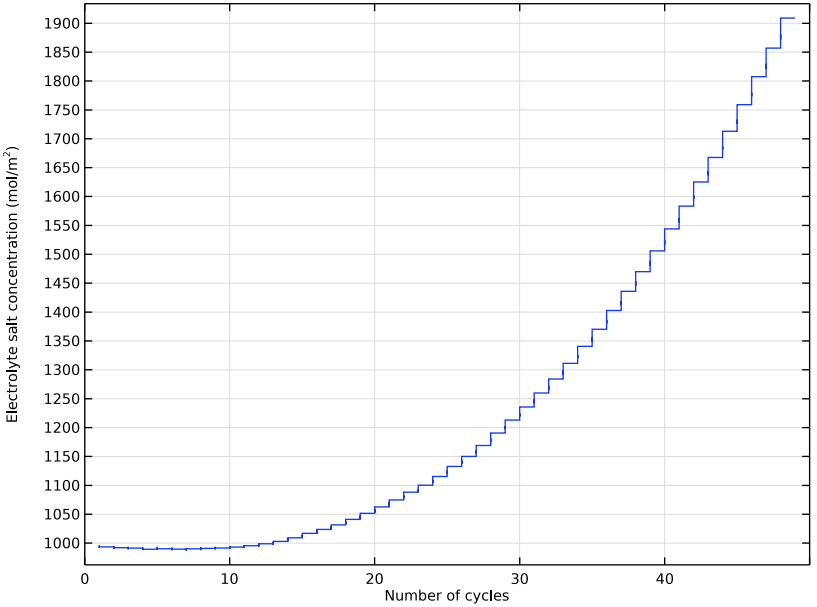

Figure 6: Electrolyte salt concentration in cell with cycling.

References

1. Y. Dai, L. Cai, and R. E. White, "Capacity Fade Model For Spinel $LiMn_2O_4$," *J. Elec. Soc.*, vol. 160, no. 1, p. A182, 2013.

Application Library path: `Battery_Design_Module/Lithium-Ion_Batteries,_Aging_and_Abuse/lmo_decomposition`

Modeling Instructions

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 (liion)**.

3 Click **Add**.

4 In the **Select Physics** tree, select **Chemical Species Transport** > **Transport of Diluted Species (tds)**.

5 Click **Add**.

6 Click **Study**.

7 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces** > **Lithium-Ion Battery** > **Time Dependent with Initialization**.

8 Click **Done**.

GLOBAL DEFINITIONS

Parameters 1

Load the parameters from a text file.

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

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

3 Click **Load from File**.

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

Draw 1D geometry of the half cell and make selections.

GEOMETRY 1

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 In the table, enter the following settings:

Coordinates (m)
0
L_sep
L_sep+L_pos

4 Click **Build All Objects**.

5 Right-click **Interval 1 (i1)** and choose **Plot**.

DEFINITIONS

Separator

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

2 In the **Settings** window for **Explicit**, type `Separator` in the **Label** text field.

3 Select Domain 1 only.

LMO

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

2 In the **Settings** window for **Explicit**, type `LMO` in the **Label** text field.

3 Select Domain 2 only.

Lithium Metal

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

2 In the **Settings** window for **Explicit**, type `Lithium Metal` in the **Label** text field.

3 Locate the **Input Entities** section. From the **Geometric entity level** list, choose **Boundary**.

4 Select Boundary 1 only.

Add material data for the electrolyte and the electrodes from the material library.

ADD MATERIAL

1 In the **Materials** 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 1:1 EC:DMC (Liquid, Li-ion Battery)**.

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

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

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

7 In the tree, select **Battery** > **Electrodes** > **Lithium Metal, Li (Negative, Li-ion Battery)**.

8 Click the **Add to Component** button in the window toolbar.

9 In the **Materials** toolbar, click **Add Material** to close the **Add Material** window.

MATERIALS

LiPF6 in 1:1 EC:DMC (Liquid, Li-ion Battery) (mat1)

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

2 From the **Selection** list, choose **Separator**.

LMO, LiMn2O4 Spinel (Positive, Li-ion Battery) (mat2)

1 In the **Model Builder** window, click **LMO, LiMn2O4 Spinel (Positive, Li-ion Battery) (mat2)**.

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

3 From the **Selection** list, choose **LMO**.

Lithium Metal, Li (Negative, Li-ion Battery) (mat3)

1 In the **Model Builder** window, click **Lithium Metal, Li (Negative, Li-ion Battery) (mat3)**.

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

3 From the **Geometric entity level** list, choose **Boundary**.

4 From the **Selection** list, choose **Lithium Metal**.

DEFINITIONS

Add model variables. Unknown variables warnings will be resolved as soon as the physics have been set up.

Variables - All Domains

1 In the **Definitions** toolbar, click **Local Variables**.

2 In the **Settings** window for **Variables**, type `Variables - All Domains` in the **Label** text field.

3 Locate the **Variables** section. Click **Load from File**.

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

Variables - LMO

1 In the **Definitions** toolbar, click **Local Variables**.

2 In the **Settings** window for **Variables**, type `Variables - LMO` in the **Label** text field.

3 Locate the **Geometric Entity Selection** section. From the **Geometric entity level** list, choose **Domain**.

4 From the **Selection** list, choose **LMO**.

5 Locate the **Variables** section. Click **Load from File**.

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

Integration LMO

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

2 In the **Settings** window for **Integration**, type `Integration LMO` in the **Label** text field.

3 In the **Operator name** text field, type `intop_lmo`.

4 Locate the **Source Selection** section. From the **Selection** list, choose **LMO**.

Integration Separator

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

2 In the **Settings** window for **Integration**, type `Integration Separator` in the **Label** text field.

3 In the **Operator name** text field, type `intop_sep`.

4 Locate the **Source Selection** section. From the **Selection** list, choose **Separator**.

Now begin defining the physics. Start with the Lithium-Ion Battery interface.

LITHIUM-ION BATTERY (LIION)

Use the **SOC and Initial Charge Distribution** node to compute initial concentration, battery cell capacity, and C-rate. The selection of the LMO electrode will be applicable once a Porous Electrode node is defined on the domain.

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 **Cell Settings** section.

3 Select the **Define cell state of charge (SOC) and initial charge inventory** checkbox.

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 **Cell Type** section.

3 From the list, choose **Half cell**.

4 Locate the **State-of-Charge Definition** section. From the list, choose **User defined**. In the $E_{\text{cell}}{}^{0}\%SOC$ text field, type `Vlow`.

5 In the $E_{\text{cell}}{}^{100}\%SOC$ text field, type `Vhigh`.

6 Locate the **Initial Cell Charge Distribution** section. In the SOC_0 text field, type `0`.

Positive Electrode Domain Selection 1

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

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

3 From the **Selection** list, choose **LMO**.

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 **Porous Matrix Properties** section.

3 In the ε_l text field, type `epsl_sep`.

Porous Electrode - LMO

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

2 In the **Settings** window for **Porous Electrode**, type `Porous Electrode - LMO` in the **Label** text field.

3 Select Domain 2 only.

4 Locate the **Electrolyte Properties** section. From the **Electrolyte material** list, choose **LiPF6 in 1:1 EC:DMC (Liquid, Li-ion Battery) (mat1)**.

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_pos0`.

7 In the ε_l text field, type `epsl_pos`.

Add a **Dissolving/Depositing Species** variable named LMO_dead. The variable represents the amount of exhausted LMO from the LMO decomposition by protons reaction.

8 Click to expand the **Dissolving–Depositing Species** section. Click **Add**.

9 In the table, enter the following settings:

Species	Density (kg/m^3)	Molar mass (kg/mol)
LMO_dead	rho_LMO	M_LMO

The electrolyte volume fraction is set as constant, that is, the molar volume of LMO is constant.

10 Clear the **Subtract volume change from electrolyte volume fraction** checkbox.

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 From the D_s list, choose **User defined**. In the associated text field, type `D_LMO`.

4 In the r_p text field, type `rp_lmo`.

Porous Electrode Reaction - Intercalation

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

2 In the **Settings** window for **Porous Electrode Reaction**, type `Porous Electrode Reaction - Intercalation` in the **Label** text field.

3 Locate the **Electrode Kinetics** section. In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0_ref_lmo`.

Add the additional reactions taking place in the porous LMO electrode domain. Treat all cations (protons) in terms of lithium ions as an assumption.

Porous Electrode - LMO

In the **Model Builder** window, click **Porous Electrode - LMO**.

Porous Electrode Reaction - Solvent Oxidation

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

2 In the **Settings** window for **Porous Electrode Reaction**, type `Porous Electrode Reaction - Solvent Oxidation` in the **Label** text field.

3 Locate the **Equilibrium Potential** section. From the E_{eq} list, choose **User defined**. In the associated text field, type `Eeq_oxid+delta_phil`.

4 Locate the **Electrode Kinetics** section. From the **Kinetics expression type** list, choose **Anodic Tafel equation**.

5 In the i_0 text field, type `i0_oxid*(cl/cl_ref)^0.5`.

6 In the A_a text field, type `Aa_oxid`.

7 Locate the **Active Specific Surface Area** section. From the **Active specific surface area** list, choose **User defined**. In the a_v text field, type `av_oxid`.

8 Locate the **Stoichiometric Coefficients** section. In the $\nu_{\mathrm{Li}\theta}$ text field, type `0`.

Porous Electrode - LMO

In the **Model Builder** window, click **Porous Electrode - LMO**.

Nonfaradaic Reactions - LMO Decomposition

1 In the **Physics** toolbar, click **Attributes** and choose **Nonfaradaic Reactions**.

2 In the **Settings** window for **Nonfaradaic Reactions**, type `Nonfaradaic Reactions - LMO Decomposition` in the **Label** text field.

3 Locate the **Reaction Rate** section. In the **Reaction rate for dissolving–depositing species** table, enter the following settings:

Species	Reaction rate (mol/(m^3*s))
LMO_dead	-Rproton

Use the **Electrode Surface**node to add all electrochemical reactions taking place on the lithium metal. Treat all cations (manganese ions and protons) in terms of lithium ions as an assumption..

Electrode Surface - Lithium Metal

1 In the **Physics** toolbar, click **Boundaries** and choose **Electrode Surface**.

2 Select Boundary 1 only.

3 In the **Settings** window for **Electrode Surface**, type `Electrode Surface - Lithium Metal` in the **Label** text field.

Electrode Reaction - Lithium

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

2 In the **Settings** window for **Electrode Reaction**, type `Electrode Reaction - Lithium` in the **Label** text field.

Electrode Surface - Lithium Metal

In the **Model Builder** window, click **Electrode Surface - Lithium Metal**.

Electrode Reaction - Manganese Deposition

1 In the **Physics** toolbar, click **Attributes** and choose **Electrode Reaction**.

2 In the **Settings** window for **Electrode Reaction**, type `Electrode Reaction - Manganese Deposition` in the **Label** text field.

3 Locate the **Equilibrium Potential** section. From the E_{eq} list, choose **User defined**. In the associated text field, type `Eeq_Mn+delta_phil`.

4 Locate the **Electrode Kinetics** section. From the **Kinetics expression type** list, choose **Cathodic Tafel equation**.

5 In the i_0 text field, type `i0_ref_Mn*cMn/cMn_ref`.

6 In the A_c text field, type `Ac_Mndep`.

7 Locate the **Stoichiometric Coefficients** section. In the n text field, type `2`.

8 In the ν_{Li+} text field, type `-2`.

Electrode Surface - Lithium Metal

In the **Model Builder** window, click **Electrode Surface - Lithium Metal**.

Electrode Reaction - Proton Reduction

1 In the **Physics** toolbar, click **Attributes** and choose **Electrode Reaction**.

2 In the **Settings** window for **Electrode Reaction**, type `Electrode Reaction - Proton Reduction` in the **Label** text field.

3 Locate the **Equilibrium Potential** section. From the E_{eq} list, choose **User defined**. In the associated text field, type `Eeq_H+delta_phil`.

4 Locate the **Electrode Kinetics** section. From the **Kinetics expression type** list, choose **Cathodic Tafel equation**.

5 In the i_0 text field, type `i0_ref_H*cH/cH_ref`.

6 In the A_c text field, type `Ac_Hred`.

Define the net cation change from the chemical reactions using a **Reaction Source** node. To do this enable **Advanced Physics Options**.

7 Click the **Show More Options** button in the **Model Builder** toolbar.

8 In the **Show More Options** dialog, in the tree, select the checkbox for the node **Physics** > **Advanced Physics Options**.

9 Click **OK**.

Reaction Source - Cation Net Chemical Reactions

1 In the **Physics** toolbar, click **Domains** and choose **Reaction Source**.

2 In the **Settings** window for **Reaction Source**, type `Reaction Source - Cation Net Chemical Reactions` in the **Label** text field.

3 Locate the **Domain Selection** section. From the **Selection** list, choose **All domains**.

4 Locate the **Reaction Source** section. In the $R_{l,src}$ text field, type `Rwater`.

Set the cell to cycle between 3.5 V and 4.5 V at C/3 with a **Charge-Discharge Cycling** node.

Charge-Discharge Cycling - Galvanic Cycling C/3

1 In the **Physics** toolbar, click **Boundaries** and choose **Charge-Discharge Cycling**.

2 In the **Settings** window for **Charge-Discharge Cycling**, type `Charge-Discharge Cycling - Galvanic Cycling C/3` in the **Label** text field.

3 Select Boundary 3 only.

4 Locate the **Discharge Settings** section. From the list, choose **C-rate multiple**.

5 In the $C_{rate,dch}$ text field, type `-Crate`.

6 In the V_{min} text field, type `Vlow`.

7 Locate the **Charge Settings** section. From the list, choose **C-rate multiple**.

8 In the $C_{rate,ch}$ text field, type `Crate`.

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

10 Locate the **Start Mode** section. From the **Start with** list, choose **Charge first**.

Continue by defining the **Transport of Diluted Species** interface that is used to model the proton, manganese ion, and water transport and reaction in the electrolyte. All fluxes related to electrochemical reactions need to be coupled to the **Lithium-Ion Battery** interface.

TRANSPORT OF DILUTED SPECIES (TDS)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Transport of Diluted Species (tds)**.

2 In the **Settings** window for **Transport of Diluted Species**, locate the **Transport Mechanisms** section.

3 Clear the **Convection** checkbox.

4 Select the **Migration in electric field** checkbox.

5 Select the **Mass transfer in porous media** checkbox.

6 Click to expand the **Dependent Variables** section. In the **Concentrations (mol/m³)** table, enter the following settings:

cH

7 Click + **Add Concentration**.

8 In the **Concentrations (mol/m³)** table, enter the following settings:

cH
cMn

9 Click + **Add Concentration**.

10 In the **Concentrations (mol/m³)** table, enter the following settings:

cH
cMn
cH2O

Species Charges

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Transport of Diluted Species (tds)** click **Species Charges**.

2 In the **Settings** window for **Species Properties**, locate the **Charge** section.

3 In the z_{cH} text field, type `zH`.

4 In the z_{cMn} text field, type `zMn`.

Porous Electrode - LMO

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

2 In the **Settings** window for **Porous Medium**, type `Porous Electrode - LMO` in the **Label** text field.

3 Locate the **Domain Selection** section. From the **Selection** list, choose **LMO**.

Fluid 1

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

2 In the **Settings** window for **Fluid**, locate the **Diffusion** section.

3 In the $D_{F,cH}$ text field, type `D_H`.

4 In the $D_{F,cMn}$ text field, type `D_Mn`.

5 In the $D_{F,cH2O}$ text field, type `D_H2O`.

6 From the **Effective diffusivity model** list, choose **Bruggeman model**.

7 Locate the **Migration in Electric Field** section. In the V text field, type `phil_ps`.

Porous Matrix 1

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

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

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

Porous Electrode Coupling 1

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

2 In the **Settings** window for **Porous Electrode Coupling**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **LMO**.

Reaction Coefficients 1

1 In the **Model Builder** window, click **Reaction Coefficients 1**.

2 In the **Settings** window for **Reaction Coefficients**, locate the **Reaction Current Source** section.

3 From the i_v list, choose **Local current source, Porous Electrode Reaction - Solvent Oxidation (liion/pce1/per2)**.

4 Locate the **Stoichiometric Coefficients** section. In the ν_{cH} text field, type `-1`.

Porous Medium - Separator

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

2 In the **Settings** window for **Porous Medium**, type `Porous Medium - Separator` in the **Label** text field.

3 Locate the **Domain Selection** section. From the **Selection** list, choose **Separator**.

Fluid 1

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

2 In the **Settings** window for **Fluid**, locate the **Diffusion** section.

3 In the $D_{F,cH}$ text field, type `D_H`.

4 In the $D_{F,cMn}$ text field, type `D_Mn`.

5 In the $D_{F,cH2O}$ text field, type `D_H2O`.

6 From the **Effective diffusivity model** list, choose **Bruggeman model**.

7 Locate the **Migration in Electric Field** section. In the V text field, type `phil_ps`.

Porous Matrix 1

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

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

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

Electrode Surface Coupling - Lithium Metal

1 In the **Physics** toolbar, click **Boundaries** and choose **Electrode Surface Coupling**.

2 In the **Settings** window for **Electrode Surface Coupling**, type `Electrode Surface Coupling - Lithium Metal` in the **Label** text field.

3 Locate the **Boundary Selection** section. From the **Selection** list, choose **Lithium Metal**.

Reaction Coefficients - Manganese deposition

1 In the **Model Builder** window, expand the **Electrode Surface Coupling - Lithium Metal** node, then click **Reaction Coefficients 1**.

2 In the **Settings** window for **Reaction Coefficients**, type `Reaction Coefficients - Manganese deposition` in the **Label** text field.

3 Locate the **Reaction Current Density** section. From the i_{loc} list, choose **Local current density, Electrode Reaction - Manganese Deposition (liion/es1/er2)**.

4 Locate the **Stoichiometric Coefficients** section. In the n text field, type `2`.

5 In the ν_{cMn} text field, type `-1`.

Electrode Surface Coupling - Lithium Metal

In the **Model Builder** window, click **Electrode Surface Coupling - Lithium Metal**.

Reaction Coefficients - Proton Reduction

1 In the **Physics** toolbar, click **Attributes** and choose **Reaction Coefficients**.

2 In the **Settings** window for **Reaction Coefficients**, type `Reaction Coefficients - Proton Reduction` in the **Label** text field.

3 Locate the **Reaction Current Density** section. From the i_{loc} list, choose **Local current density, Electrode Reaction - Proton Reduction (liion/es1/er3)**.

4 Locate the **Stoichiometric Coefficients** section. In the ν_{cH} text field, type `-1`.

The last step is to define the chemical reactions in **Reaction** nodes.

Reactions - LMO

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

2 In the **Settings** window for **Reactions**, type `Reactions - LMO` in the **Label** text field.

3 Locate the **Domain Selection** section. From the **Selection** list, choose **LMO**.

4 Locate the **Reaction Rates** section. In the R_{cH} text field, type `-4*Rproton+2*Rwater`.

5 In the R_{cMn} text field, type `Rproton`.

6 In the R_{cH2O} text field, type `2*Rproton-Rwater`.

Reactions - Separator

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

2 In the **Settings** window for **Reactions**, type `Reactions - Separator` in the **Label** text field.

3 Locate the **Domain Selection** section. From the **Selection** list, choose **Separator**.

4 Locate the **Reaction Rates** section. In the R_{cH} text field, type `2*Rwater`.

5 In the R_{cH2O} text field, type `-Rwater`.

Add multiple time-dependent study steps to refine the results of the first and last cycle.

STUDY 1

Step 3: Time Dependent 1

In the **Model Builder** window, under **Study 1** right-click **Step 2: Time Dependent** and choose **Duplicate**.

Step 4: Time Dependent 2

In the **Model Builder** window, right-click **Step 3: Time Dependent 1** and choose **Duplicate**.

Time Dependent - First Cycle

1. In the **Settings** window for **Time Dependent**, type `Time Dependent - First Cycle` in the **Label** text field.
2. Locate the **Study Settings** section. From the **Time unit** list, choose **h**.
3. In the **Output times** text field, type `0 7`.

Time Dependent - Cycling

1. In the **Model Builder** window, under **Study 1** click **Step 3: Time Dependent 1**.
2. In the **Settings** window for **Time Dependent**, type `Time Dependent - Cycling` in the **Label** text field.
3. Locate the **Study Settings** section. From the **Time unit** list, choose **h**.
4. In the **Output times** text field, type `range(0,0.5,300)`.

Time Dependent - Last Cycle

1. In the **Model Builder** window, under **Study 1** click **Step 4: Time Dependent 2**.
2. In the **Settings** window for **Time Dependent**, type `Time Dependent - Last Cycle` in the **Label** text field.
3. Locate the **Study Settings** section. From the **Time unit** list, choose **h**.
4. In the **Output times** text field, type `0 7`.

Solution 1 (sol1)

1. In the **Study** toolbar, click **Show Default Solver**.
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.cycle_no>0`	True (>=1)	√	`Stop expression 1`

9 Locate the **Output at Stop** section. Clear the **Add information** checkbox.

10 In the **Model Builder** window, under **Study 1** > **Solver Configurations** > **Solution 1 (sol1)** right-click **Time-Dependent Solver 2** and choose **Stop Condition**.

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

12 Click + **Add**.

13 In the table, enter the following settings:

Stop expression	Stop if	Active	Description
`comp1.cycle_no>48`	True (>=1)	√	`Stop expression 1`

14 Locate the **Output at Stop** section. Clear the **Add information** checkbox.

15 In the **Model Builder** window, under **Study 1** > **Solver Configurations** > **Solution 1 (sol1)** click **Time-Dependent Solver 3**.

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

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

18 Right-click **Study 1** > **Solver Configurations** > **Solution 1 (sol1)** > **Time-Dependent Solver 3** and choose **Stop Condition**.

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

20 Click + **Add**.

21 In the table, enter the following settings:

Stop expression	Stop if	Active	Description
`comp1.cycle_no>49`	True (>=1)	√	`Stop expression 1`

22 Locate the **Output at Stop** section. Clear the **Add information** checkbox.

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

RESULTS

Cell Voltage

The following steps produce the plot groups and images in the model documentation.

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

2 Locate the **Data** section. From the **Dataset** list, choose **Study 1/Solution Store 3 (sol4)**.

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

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

5 Select the **y-axis label** checkbox. In the associated text field, type `Cell voltage (V)`.

6 Locate the **Legend** section. Clear the **Show legends** checkbox.

Global 1

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

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

3 From the **Parameter** list, choose **Expression**.

4 In the **Expression** text field, type `t+t_cycle_first`.

5 From the **Unit** list, choose **h**.

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

Cell and Average Electrode Cell State of Charge (liion)

1 In the **Model Builder** window, under **Results** click **Cell and Average Electrode Cell State of Charge (liion)**.

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

3 From the **Dataset** list, choose **Study 1/Solution Store 3 (sol4)**.

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

Global 1

1 In the **Model Builder** window, expand the **Cell and Average Electrode Cell State of Charge (liion)** node, then click **Global 1**.

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+t_cycle_first`.

5 From the **Unit** list, choose **h**.

Global 2

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

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+t_cycle_first`.

5 From the **Unit** list, choose **h**.

6 In the **Cell and Average Electrode Cell State of Charge (liion)** toolbar, click **Plot**.

Some of the default plots are redundant for the scope of this example and can be removed.

Concentration, H (tds), Concentration, H2O (tds), Concentration, Mn (tds), Concentrations, All Species (tds), Electrode Potential with Respect to Adjacent Reference

(liion), Electrolyte Salt Concentration (liion), Particle Surface State of Charge (liion), Volumetric Current Density (liion)

1 In the **Model Builder** window, under **Results**, Ctrl-click to select **Electrode Potential with Respect to Adjacent Reference (liion)**, **Electrolyte Salt Concentration (liion)**, **Volumetric Current Density (liion)**, **Particle Surface State of Charge (liion)**, **Concentrations, All Species (tds)**, **Concentration, H (tds)**, **Concentration, Mn (tds)**, and **Concentration, H2O (tds)**.

2 Right-click and choose **Delete**.

Cell Capacity

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

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

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/Solution Store 3 (sol4)**.

4 Locate the **Title** section. From the **Title type** list, choose **None**.

5 Locate the **Plot Settings** section. Select the **x-axis label** checkbox.

6 Locate the **Legend** section. Clear the **Show legends** checkbox.

Global 1

1 Right-click **Cell Capacity** 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)** > **Lithium-Ion Battery** > **liion.Q_cell - Battery cell capacity - C**.

3 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
`liion.Q_cell`	`Ah`	`Battery cell capacity`

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

5 In the **Expression** text field, type `t+t_cycle_first`.

6 From the **Unit** list, choose **h**.

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

Electrode Volume Fraction

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

2 In the **Settings** window for **1D Plot Group**, type `Electrode Volume Fraction` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/Solution Store 3 (sol4)**.

4 Locate the **Title** section. From the **Title type** list, choose **None**.

5 Locate the **Legend** section. Clear the **Show legends** checkbox.

Global 1

1 In the **Electrode Volume Fraction** toolbar, click **Global**.

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

3 In the table, enter the following settings:

Expression	Unit	Description
epss_LMO_pos	1	Electrode volume fraction in the positive electrode

4 Click **Replace Expression** in the upper-right corner of the **x-Axis Data** section. From the menu, choose **Component 1 (comp1)** > **Lithium-Ion Battery** > **Charge-Discharge Cycling - Galvanic Cycling C/3** > **liion.cdc1.cycle_counter - Number of cycles**.

5 In the **Electrode Volume Fraction** toolbar, click **Plot**.

Diffusion Coefficient in LMO Particles

1 In the **Model Builder** window, right-click **Electrode Volume Fraction** and choose **Duplicate**.

2 In the **Settings** window for **1D Plot Group**, type `Diffusion Coefficient in LMO Particles` in the **Label** text field.

3 Locate the **Plot Settings** section.

4 Select the **y-axis label** checkbox. In the associated text field, type `Diffusion coefficient LMO (m<sup>2</sup>/s)`.

Global 1

1 In the **Model Builder** window, expand the **Diffusion Coefficient in LMO Particles** node, then click **Global 1**.

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

3 In the table, enter the following settings:

Expression	Unit	Description
D_LMO_pos	m^2/s	Diffusion coefficient of lithium within LMO particles in the positive electrode

4 In the **Diffusion Coefficient in LMO Particles** toolbar, click **Plot**.

Discharge Curve Comparison

1 In the **Model Builder** window, right-click **Diffusion Coefficient in LMO Particles** and choose **Duplicate**.

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

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

4 Locate the **Plot Settings** section.

5 Select the **x-axis label** checkbox. In the associated text field, type `Discharge time (s)`.

6 In the **y-axis label** text field, type `Cell voltage (V)`.

7 Locate the **Legend** section. Select the **Show legends** checkbox.

Global 1

1 In the **Model Builder** window, expand the **Discharge Curve Comparison** node, then click **Global 1**.

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

3 From the **Dataset** list, choose **Study 1/Solution Store 2 (sol3)**.

4 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)** > **Lithium-Ion Battery** > **Charge-Discharge Cycling - Galvanic Cycling C/3** > **liion.cdc1.phis0 - Cell potential - V**.

5 Locate the **x-Axis Data** section. In the **Expression** text field, type `t_cycle_dch_first`.

6 Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.

7 Click to expand the **Legends** section. From the **Legends** list, choose **Manual**.

8 In the table, enter the following settings:

Legends
1st cycle

Filter 1

1 Right-click **Global 1** and choose **Filter**.

2 In the **Settings** window for **Filter**, locate the **Line Segment Selection** section.

3 Clear the **Decreasing x** checkbox.

4 Clear the **Increasing y** checkbox.

Global 2

1 Right-click **Global 1** and choose **Duplicate**.

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

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

4 Locate the **x-Axis Data** section. In the **Expression** text field, type `t_cycle_dch_last`.

5 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Solid**.

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

Legends
50th cycle

7 In the **Discharge Curve Comparison** toolbar, click **Plot**.

Capacity vs. Cycle Number

1 In the **Model Builder** window, right-click **Diffusion Coefficient in LMO Particles** and choose **Duplicate**.

2 In the **Settings** window for **1D Plot Group**, type `Capacity vs. Cycle Number` in the **Label** text field.

3 Locate the **Plot Settings** section. In the **y-axis label** text field, type `Relative capacity (-)`.

4 Locate the **Legend** section. Select the **Show legends** checkbox.

5 From the **Position** list, choose **Lower left**.

Global 1

1 In the **Model Builder** window, expand the **Capacity vs. Cycle Number** node, then click **Global 1**.

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)** > **Lithium-Ion Battery** > **liion.SOH_cell - Cell state of health - 1**.

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

4 In the table, enter the following settings:

Legends
Based on cyclable lithium and host capacity

Global 2

1 Right-click **Results** > **Capacity vs. Cycle Number** > **Global 1** and choose **Duplicate**.

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

3 In the table, enter the following settings:

Expression	Unit	Description
(t-liion.cdc1.t_dch_start)/t_cycle_first	1	

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

Legends
Nominal C/3 discharge capacity

Filter 1

1 Right-click **Global 2** and choose **Filter**.

2 In the **Settings** window for **Filter**, locate the **Line Segment Selection** section.

3 Clear the **Decreasing x** checkbox.

4 In the **Capacity vs. Cycle Number** toolbar, click **Plot**.

Electrolyte Salt Concentration in Battery

1 In the **Model Builder** window, right-click **Diffusion Coefficient in LMO Particles** and choose **Duplicate**.

2 In the **Settings** window for **1D Plot Group**, type `Electrolyte Salt Concentration in Battery` in the **Label** text field.

3 Locate the **Plot Settings** section. In the **y-axis label** text field, type `Electrolyte salt concentration (mol/m<sup>2</sup>)`.

Global 1

1 In the **Model Builder** window, expand the **Electrolyte Salt Concentration in Battery** node, then click **Global 1**.

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

3 In the table, enter the following settings:

Expression	Unit	Description
cl_battery	mol/m^3	Net lithium ion concentration in battery

4 In the **Electrolyte Salt Concentration in Battery** toolbar, click **Plot**.