Model created in COMSOL Multiphysics 6.4

Copper Current-Collector Dissolution

Introduction

The copper current collector on negative graphite electrodes in lithium-ion batteries have been seen to dissolve at over-discharge. This can be a safety concern as the dissolution damages the current collector irreversibly and dissolved copper ions can redeposit and form dendrites. Batteries are usually operated within specified voltage limits, either on cell or pack level, in order to avoid over-discharge. However, over-discharge may still occur, either in a pack due to charge imbalances between the individual cells, or, as we will partly investigate in this tutorial, due to local heterogeneities in the electrodes within a single battery cell.

This tutorial investigates the copper current-collector dissolution during over-discharge from an electrode with an inhomogeneous graphite electrode material coating. The cuprous ion concentration, as well as the redeposited copper distribution in the cell, are predicted.

Model Definition

GENERAL

The model is set up in 2D for a graphite/NMC battery cell with a 1.0 M $LiPF_6$ in EC:EMC (3:7 by weight) electrolyte. Properties for these materials are taken from the Battery material library.

The model consists of the following three domains:

- Negative porous electrode: Graphite (MCMB Li_xC_6) active material (~64 µm).
- Separator (25 µm).
- Positive porous electrode: NMC 811 active material (40 µm).

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

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

More information about how to use the Lithium-Ion Battery interface can be found in the 1D Isothermal Lithium-Ion Battery example.

The Transport of Diluted Species interface is used to define the copper (cuprous) ion reaction and transport in the cell. Additional features in the Lithium-Ion Battery interface are used to define the electrochemical copper dissolution/deposition reaction (as described below).

The model is solved for two shapes of dents in the graphite active material coating. Figure 1 displays the two shapes of dents investigated.

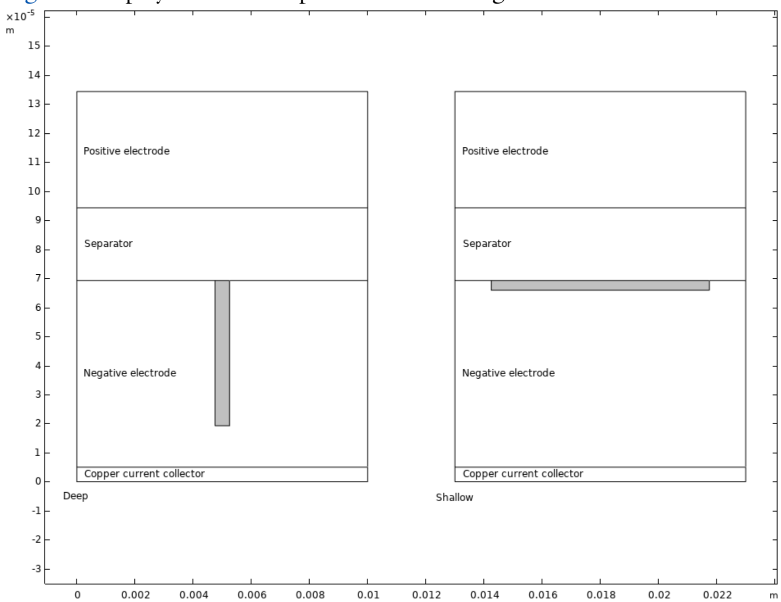

Figure 1: The 2D model geometry. Two dent shapes (gray) with the same volume are studied.

ELECTROLYTE PHASE POTENTIAL DEFINITIONS

In this model we assume the cuprous ion concentration to be low in relation to the Li^+/ PF_6^- (+ solvent) electrolyte, and assume a dilute approximation of the Cu^+ transport and electrochemical reactions to be valid. We will hence assume that the electrolyte phase potential field is governed by the lithium-ion transport, and that the contribution to the electrolyte potential field from the cuprous ion transport may be neglected.

A caveat here is that the electrolyte phase potential variable ϕ_l solved for by the Lithium-Ion Battery interface is defined by concentrated electrolyte theory, where ϕ_l is defined with reference to a Li^+/Li(s) electrode of the same local concentration c_l of lithium ions, also solved for by the Lithium-Ion Battery interface. We need hence to correct for the local lithium concentration before we can use the electrolyte phase potential variable as input to the cuprous reaction and transport terms. With the absence of concentration dependent Li^+ activities, an ideal electrolyte concentration dependence for single charged ions is used as an approximation, as follows:

$$\Delta\phi_l = -\frac{RT}{F}\ln\left(\frac{c_l}{c_{l,\mathrm{ref}}}\right) \tag{1}$$

where $c_{l,\mathrm{ref}}$ refers to a chosen (1 M) reference salt-concentration of the battery electrolyte.

A pseudo-potentiostatic electrolyte potential, $\phi_{l,\mathrm{ps}}$ (V), to be used for the cuprous ion transport and kinetic definitions can now be defined as:

$$\phi_{l,\,\mathrm{ps}} = \phi_l + \Delta\phi_l \tag{2}$$

COPPER DISSOLUTION/DEPOSITION REACTION

On the negative porous electrode, the copper reaction is defined as an additional reaction to the main graphite-lithium intercalation reaction. This is done using an additional **Porous Electrode Reaction** in the **Porous Electrode** node for the negative electrode. At the copper current-collector boundary, the reaction is added as an **Electrode Reaction** in an **Internal Electrode Surface** node.

The reaction is reversible, purely electrochemical, and considers cuprous ions (Ref. 1):

$$\mathrm{Cu(s)} \leftrightarrow \mathrm{Cu}^+ + \mathrm{e}^-$$

The electrochemical reaction current, i_{Cu}, is defined by concentration-dependent Butler–Volmer kinetics (Ref. 2):

$$i_{\mathrm{Cu}} = i_{0,\,\mathrm{ref}}\left(F_a\exp\left(\frac{F\eta_{\mathrm{Cu}}}{2RT}\right) - F_c\exp\left(-\frac{F\eta_{\mathrm{Cu}}}{2RT}\right)\right) \tag{3}$$

where the pre-exponential factors for the anodic, F_{a}, and cathodic, F_{c}, terms are defined as

$$\begin{aligned}
F_{\mathrm{a}} &= \frac{c_{\mathrm{Cu(s)}}}{c_{\mathrm{Cu(s),cov}}} \quad &\text{if} \quad \frac{c_{\mathrm{Cu(s)}}}{c_{\mathrm{LiCu(s),cov}}} \le 1\\
F_{\mathrm{a}} &= 1 \quad &\text{if} \quad \frac{c_{\mathrm{Cu(s)}}}{c_{\mathrm{Cu(s),cov}}} > 1\\
F_{\mathrm{c}} &= \frac{c_{\mathrm{Cu}}}{c_{\mathrm{Cu,\,ref}}}
\end{aligned} \tag{4}$$

In the expressions above:

- $i_{0,\mathrm{ref}}$ is the reference exchange current density.
- c_{Cu} is the cuprous ion concentration in the electrolyte.
- $c_{\mathrm{Cu,ref}}$ is the reference cuprous ion concentration, set to 1 M.
- $c_{\mathrm{Cu(s),cov}}$ is the concentration of a monolayer fully covered with deposited copper on the negative active material. The monolayer thickness is set to 0.1 nm.
- $c_{\mathrm{Cu(s)}}$ is the deposited copper concentration (equal to $c_{\mathrm{Cu(s),cov}}$ at the current-collector boundary).
- η_{Cu} is the overpotential of the copper reaction with the equilibrium potential, $E_{\mathrm{eq,Cu}}$, set to 3.5 V versus $Li^+/Li(s)$ in a 1M Li^+/PF_6^- electrolyte.:

$$\eta_{\mathrm{Cu}} = \phi_{\mathrm{s}} - \phi_{\mathrm{l,ps}} - E_{\mathrm{eq,\,Cu}} \tag{5}$$

The deposited copper concentration is computed using the in-built **Dissolving–Depositing Species** feature in the main Porous Electrode node. The equation that is solved takes the following form for the copper reaction:

$$\frac{\mathrm{d}c_{\mathrm{Cu(s)}}}{\mathrm{d}t} = \frac{-a_v i_{\mathrm{Cu}}}{F} \tag{6}$$

where a_v is the specific surface area (m^2/m^3) of the active material particles.

COPPER FLUX AND MASS TRANSPORT

In the Lithium-ion Battery interface, the flux to/from the copper reaction site is assumed to be in the form of lithium ions to maintain charge neutrality and binary salt transport conditions in the electrolyte.

The Transport of Diluted Species interface solves for the transport of cuprous ions by diffusion and migration. For the migration term, the electrolyte potential $\phi_{\mathrm{l,ps}}$ is used, as defined above. On the copper current collector boundary, the flux due to dissolution of copper is computed using an **Electrode Surface Coupling** node. At the negative porous electrode, the **Porous Electrode Coupling** node defines the redeposition of copper. Both these coupling nodes refer to the electrochemical reactions defined in the Lithium-Ion Battery Interface.

With the definitions above, the net electrolyte salt concentration, $c_{\mathrm{l,net}}$, is given by the difference in electrolyte salt concentration, c_{l}, as computed by the Lithium-Ion Battery interface and the cuprous ion concentration:

$$c_{\mathrm{l,net}} = c_{\mathrm{l}} - c_{\mathrm{Cu}} \tag{7}$$

Results and Discussion

A galvanostatic cell discharge between 4.1 V and –0.05 V is modeled to capture the overdischarge behavior. In Figure 2, the cell voltage and cuprous ion concentration in the cell is shown near the end of the discharge. The voltage is well below the normal lower cutoff voltage (~2.7 V) when the amount of cuprous ions starts to increase. The results are similar for both dent shapes.

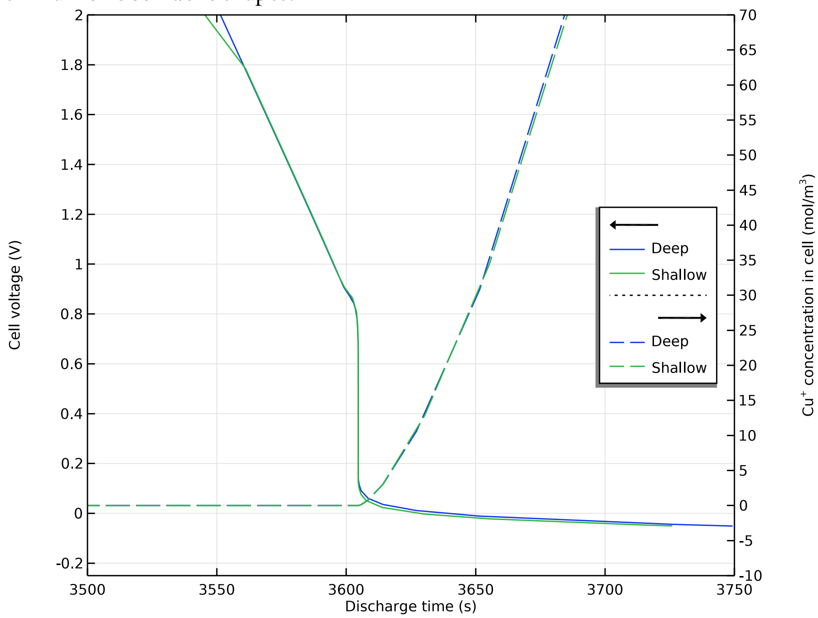

Figure 2: Cell voltage and cuprous ion concentration in the cell near the end of the discharge for the two dent shapes.

In Figure 3, the electrode potential distribution in the porous electrodes are shown at the time when the potential is higher than 3.5 V in the negative electrode at the copper current collector.

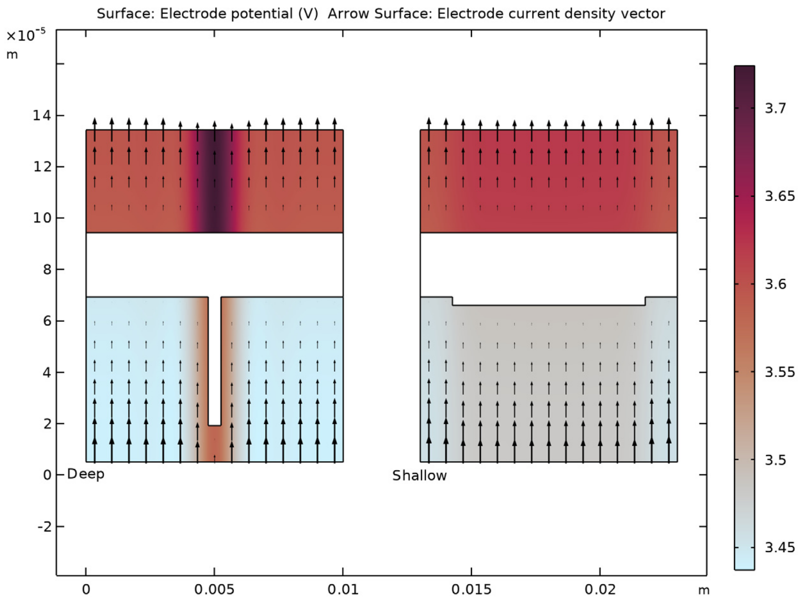

Figure 3: Electrode potential distribution once local negative electrode potential is higher than 3.5 V at the copper current collector (~3605 s).

As shown in Figure 4, this marks the initiation of copper dissolution and correlates to the copper reaction equilibrium potential set to 3.5 V in the model. Comparing the two different dent shapes shows that the deeper dent contributes to a more uneven potential distribution and copper dissolution.

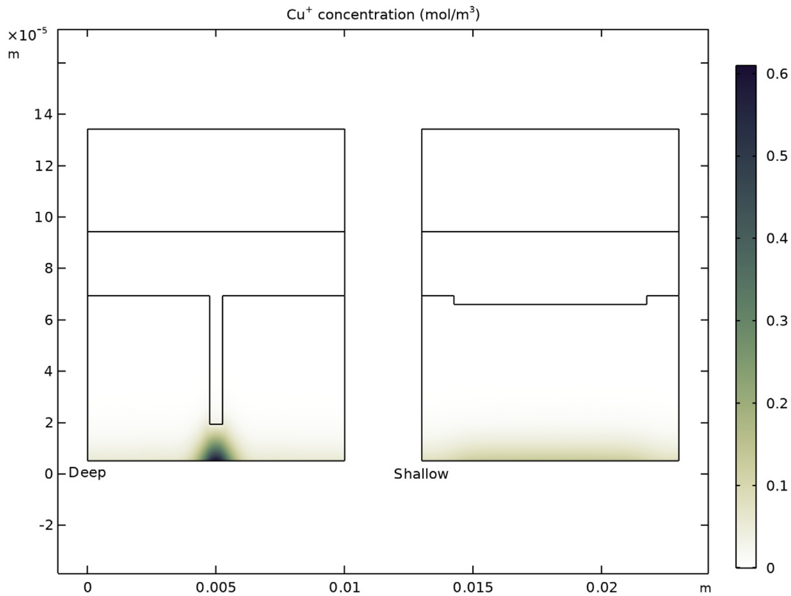

Figure 4: Cuprous ion concentration in the cell once local negative electrode potential is higher than 3.5 V at the copper current collector (~3605 s).

The dissolved cuprous ions will redeposit at lower local electrode potentials. This can be a safety concern, for instance, if the deposits take the form of dendrites. The deposited copper concentrations at –0.05 V (soon after battery polarity reversal) are displayed in Figure 5. Higher local concentrations and more uneven distribution are shown for the deeper dent.

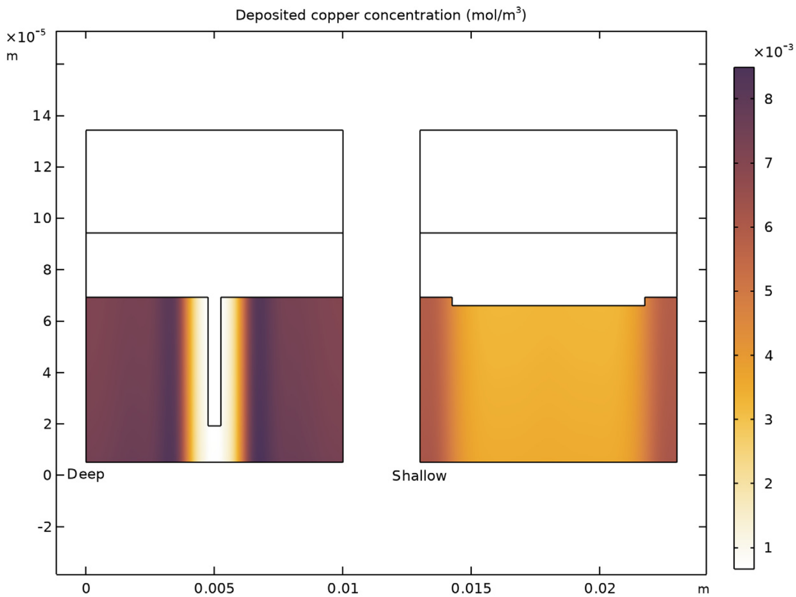

Figure 5: The deposited copper concentration at -0.05 V cell voltage.

The dissolution current along the copper current collector is displayed in Figure 6. Faster dissolution of the current collector is shown beneath the tip of the dent. Results point to higher risk of local damage for the deep dent.

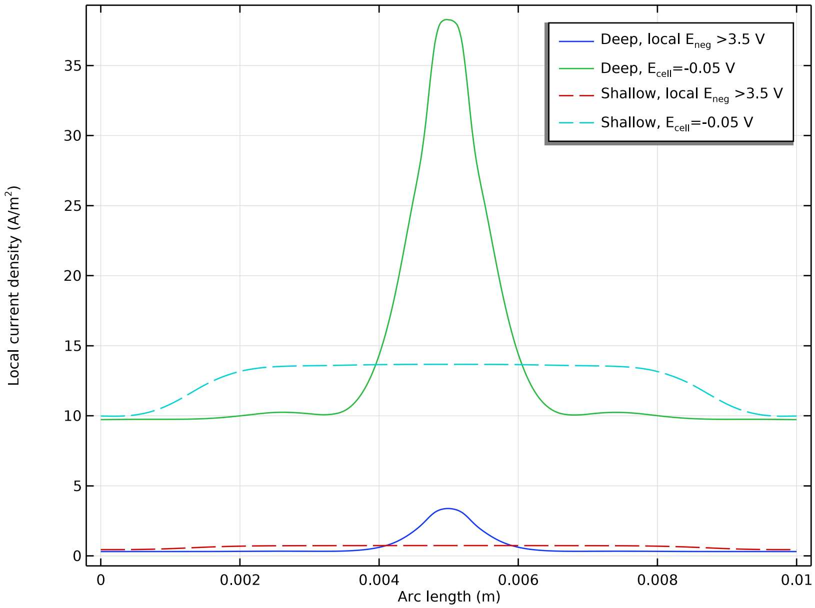

Figure 6: Copper dissolution current at the copper current collector boundary once local negative electrode potential is higher than 3.5 V at the copper current collector (~3605 s) and at cell voltage -0.05 V.

References

1. L. Guo, D.B. Thornton, M.A. Kanonfel, I.E.L. Stephens, and M.P. Ryan, "Degradation in lithium ion battery current collectors," *J. Phys. Energy*., vol. 3, pp. 2874, 2000.

2. S.E.J. O'Kane, I.D. Campbell, M.W.J. Marzook, G.J. Offer, and M. Marinescu, "Physical Origin of the Differential Voltage Minimum Associated with Lithium Plating in Li-Ion Batteries," *J. Elec. Soc.*, vol. 167, pp. 090540, 2020.

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

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 **2D**.
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 `cu_current_collector_dissolution_parameters.txt`.

Add material data for the electrolyte, the electrodes, and the copper current collector 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 > Graphite, LixC6 MCMB (Negative, Li-ion Battery)**.

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

7 In the tree, select **Battery > Electrodes > NMC 811, LiNi0.8Mn0.1Co0.1O2 (Positive, Li-ion Battery)**.

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

9 In the tree, select **Built-in > Copper**.

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

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

GEOMETRY 1

Draw the model geometry in 2D to investigate different shapes of dents.

Rectangle 1 (r1)

1 In the **Geometry** toolbar, click **Rectangle**.

2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.

3 In the **Width** text field, type `w_battery`.

4 In the **Height** text field, type `L_neg_cc`.

Rectangle 2 (r2)

1 In the **Geometry** toolbar, click **Rectangle**.

2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.

3 In the **Width** text field, type `w_battery`.

4 In the **Height** text field, type `L_neg`.

5 Locate the **Position** section. In the **y** text field, type `L_neg_cc`.

Rectangle 3 (r3)

1 In the **Geometry** toolbar, click **Rectangle**.

2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.

3 In the **Width** text field, type `w_battery`.

4 In the **Height** text field, type `L_sep`.

5 Locate the **Position** section. In the **y** text field, type `L_neg_cc+L_neg`.

Rectangle 4 (r4)

1 In the **Geometry** toolbar, click **Rectangle**.

2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.

3 In the **Width** text field, type `w_battery`.

4 In the **Height** text field, type `L_pos`.

5 Locate the **Position** section. In the **y** text field, type `L_neg_cc+L_neg+L_sep`.

Rectangle 5 (r5)

1 In the **Geometry** toolbar, click **Rectangle**.

2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.

3 In the **Width** text field, type `w_dent`.

4 In the **Height** text field, type `depth_dent`.

5 Locate the **Position** section. In the **x** text field, type `w_battery/2-w_dent/2`.

6 In the **y** text field, type `L_neg+L_neg_cc-depth_dent`.

7 In the **Home** toolbar, click **Build All**.

DEFINITIONS

In the **Model Builder** window, expand the **Component 1 (comp1)** > **Definitions** node.

View 1

Use the View node to scale the geometry in the **Graphics** window to better visualize the drawn domains.

Axis

1 In the **Model Builder** window, expand the **Component 1 (comp1)** > **Definitions** > **View 1** node, then click **Axis**.

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

3 From the **View scale** list, choose **Manual**.

4 In the **y scale** text field, type `100`.

5 Click **Update**.

6 Click the **Zoom Extents** button in the **Graphics** toolbar.

Add selections to facilitate building the model.

Negative Electrode

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

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

3 Select Domain 2 only.

Positive Electrode

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

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

3 Select Domain 4 only.

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 3 only.

Dent

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

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

3 Select Domain 5 only.

Copper Current Collector

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

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

3 Select Domain 1 only.

Copper Current-Collector Boundary

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

2 In the **Settings** window for **Explicit**, type `Copper Current-Collector Boundary` in the **Label** text field.

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

4 Select Boundary 4 only.

Aluminum Current-Collector Boundary

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

2 In the **Settings** window for **Explicit**, type `Aluminum Current-Collector Boundary` in the **Label** text field.

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

4 Select Boundary 9 only.

Integration - Electrolyte-Filled Domains

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

Create an integration operator for all electrolyte filled domains to compute, for example, the total amount of cuprous ions in the cell.

2 In the **Settings** window for **Integration**, type `Integration - Electrolyte-Filled Domains` in the **Label** text field.

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

4 Select Domains 2–5 only.

Now assign the previously added materials to the different domains of the geometry.

MATERIALS

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

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Materials** click **LiPF6 in 1:1 EC:DMC (Liquid, Li-ion Battery) (mat1)**.

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

3 Click **Clear Selection**.

4 Select Domains 3 and 5 only.

Graphite, LixC6 MCMB (Negative, Li-ion Battery) (mat2)

1 In the **Model Builder** window, click **Graphite, LixC6 MCMB (Negative, Li-ion Battery) (mat2)**.

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

3 From the **Selection** list, choose **Negative Electrode**.

NMC 811, LiNi0.8Mn0.1Co0.1O2 (Positive, Li-ion Battery) (mat3)

1 In the **Model Builder** window, click **NMC 811, LiNi0.8Mn0.1Co0.1O2 (Positive, Li-ion Battery) (mat3)**.

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

3 From the **Selection** list, choose **Positive Electrode**.

Copper (mat4)

1 In the **Model Builder** window, click **Copper (mat4)**.

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

3 From the **Selection** list, choose **Copper Current Collector**.

DEFINITIONS

Add model variables.

Variables 1

1 In the **Definitions** toolbar, click **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 `cu_current_collector_dissolution_variables.txt`.

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

LITHIUM-ION BATTERY (LIION)

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`.

Electrolyte 1

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

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

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

Current Conductor 1

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

2 In the **Settings** window for **Current Conductor**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Copper Current Collector**.

Porous Electrode - Negative

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

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

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

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_neg`.

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

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

8 Locate the **Effective Transport Parameter Correction** section. From the **Electric conductivity** list, choose **No correction**.

In the negative electrode, add copper metal as dissolving–depositing species.

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

10 In the table, enter the following settings:

Species	**Density (kg/m^3)**	**Molar mass (kg/mol)**
CuMetal	rho_Cu	M_Cu

11 Clear the **Add volume change to electrode volume fraction** checkbox.

12 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 **Species Settings** section.
3. In the $c_{s,init}$ text field, type `cs_init_neg`.
4. Locate the **Particle Transport Properties** section. In the r_p text field, type `rp_neg`.

Porous Electrode Reaction - Intercalation

1. In the **Model Builder** window, under **Component 1 (comp1)** > **Lithium-Ion Battery (liion)** > **Porous Electrode - Negative** 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_neg`.

Porous Electrode Reaction - Copper

1. Right-click **Porous Electrode Reaction - Intercalation** and choose **Duplicate**.

   Define the copper dissolution/deposition reaction in an additional Porous Electrode Reaction node. To maintain electrolyte neutrality and binary conditions in the interface, cuprous ions are assumed to behave as lithium ions; that is, the copper reaction introduces a flux of lithium ions.

2. In the **Settings** window for **Porous Electrode Reaction**, type `Porous Electrode Reaction - Copper` 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_Cu+delta_phil`.
4. Locate the **Electrode Kinetics** section. From the **Kinetics expression type** list, choose **Concentration dependent kinetics**.
5. In the i_0 text field, type `i0_ref_CuMetal`.
6. In the C_R text field, type `min(liion.c_pce1_CuMetal/(cCucov*liion.Av_pce1_per2),1)`.
7. In the C_O text field, type `cCu/cCu_ref`.

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

9 In the **Stoichiometric coefficients for dissolving–depositing species:** table, enter the following settings:

Species	Stoichiometric coefficient (1)
CuMetal	1

Porous Electrode - Positive

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

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

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

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_pos`.

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

8 Locate the **Effective Transport Parameter Correction** section. From the **Electric conductivity** list, choose **No correction**.

Particle Intercalation 1

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

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

3 In the $c_{s,init}$ text field, type `cs_init_pos`.

4 Locate the **Particle Transport Properties** section. In the r_p text field, type `rp_pos`.

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 $i_{0,ref}(T)$ text field, type `i0_ref_pos`.

At the boundary between the copper current-collector and the porous negative electrode, define the copper dissolution/deposition reaction. In contrast to the porous electrode, the metallic copper amount can be set as constant.

Internal Electrode Surface - Copper

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

2 In the **Settings** window for **Internal Electrode Surface**, type `Internal Electrode Surface - Copper` in the **Label** text field.

3 Locate the **Boundary Selection** section. From the **Selection** list, choose **Copper Current-Collector Boundary**.

Electrode Reaction 1

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

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

3 From the **Material** list, choose **Graphite, LixC6 MCMB (Negative, Li-ion Battery) (mat2)**.

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

5 Locate the **Electrode Kinetics** section. From the **Kinetics expression type** list, choose **Concentration dependent kinetics**.

6 In the i_0 text field, type `i0_ref_CuMetal`.

7 In the C_O text field, type `cCu/cCu_ref`.

Electric Ground 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Electric Ground**.

2 Select Boundary 2 only.

Electrode Current 1

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

2 In the **Settings** window for **Electrode Current**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Aluminum Current-Collector Boundary**.

4 Locate the **Electrode Current** section. In the $I_{s,total}$ text field, type `-I_1C_cell`.

To improve the initialization of the computations set the approximate potential (~cell voltage) in the positive electrode. This is necessary due to the highly nonlinear copper reaction kinetics.

Initial Values 2

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

2 Select Domain 4 only.

3 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

4 In the *phis* text field, type `V0`.

Continue by defining the Transport of Diluted Species interface that is used to track the cuprous ion movement in the electrolyte. All fluxes due to copper dissolution/deposition needs 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 **Domain Selection** section.

3 In the list box, select **1**.

4 Click **Remove from Selection**.

5 Select Domains 2–5 only.

6 Locate the **Transport Mechanisms** section. Clear the **Convection** checkbox.

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

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

9 Click to expand the **Dependent Variables** section. In the **Concentrations (mol/m^3)** table, enter the following settings:

`cCu`

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_{cCu} text field, type `zCu`.

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_{cCu} text field, type `D_Cu`.

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

Electrode Surface Coupling - Copper

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 - Copper` in the **Label** text field.

3 Locate the **Boundary Selection** section. From the **Selection** list, choose **Copper Current-Collector Boundary**.

Reaction Coefficients 1

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

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

3 From the i_{loc} list, choose **Local current density, Electrode Reaction 1 (liion/bei1/er1)**.

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

Porous Electrode - Negative

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

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

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

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 $D_{F,cCu}$ text field, type `D_Cu`.

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

5 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_neg`.

Porous Electrode - Positive

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

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

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

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 $D_{F,cCu}$ text field, type `D_Cu`.

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

5 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`.

Separator

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

2 In the **Settings** window for **Porous Medium**, type `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 $D_{F,cCu}$ text field, type `D_Cu`.

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

5 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`.

Porous Electrode Coupling - Copper

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

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

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

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 - Copper (liion/pce1/per2)**.

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

The highly nonlinear copper reaction kinetics require the steps in the study to set different initial cuprous ion concentrations to initialize the computations. Use an additional Initial Values node for this purpose.

Initial Values 2

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

2 In the **Settings** window for **Initial Values**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **All domains**.

4 Locate the **Initial Values** section. In the cCu text field, type cCu0.

MESH 1

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Mesh 1**.

2 In the **Settings** window for **Mesh**, locate the **Sequence Type** section.

3 From the list, choose **User-controlled mesh**.

Size 1

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Mesh 1** click **Size 1**.

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

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

4 Select Boundaries 4, 6, 10, 11, 13, and 14 only.

5 Locate the **Element Size** section. From the **Predefined** list, choose **Extremely fine**.

Free Triangular 1

1 In the **Model Builder** window, click **Free Triangular 1**.

2 In the **Settings** window for **Free Triangular**, click to expand the **Scale Geometry** section.

3 In the **y-direction scale** text field, type 50.

4 Click **Build All**.

STUDY 1

Use a parametric sweep to study the copper dissolution for two geometrical shapes of dents.

Parametric Sweep

1 In the **Study** toolbar, click **Parametric Sweep**.

2 In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.

3 Click + **Add**.

4 Click + **Add**.

5 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
w_dent (Width of dent in negative electrode coating)	`0.5[mm] 7.5[mm]`	`m`
depth_dent (Dent depth in negative active material)	`50[um] 20[um]/6`	`m`

The cuprous ion concentration needs to be zero in Step 1. The second step runs smoother with nonzero concentration. Use the Modify model configuration support to achieve this.

Step 1: Current Distribution Initialization

1 In the **Model Builder** window, click **Step 1: Current Distribution Initialization**.

2 In the **Settings** window for **Current Distribution Initialization**, locate the **Study Settings** section.

3 From the **Current distribution type** list, choose **Secondary**.

4 Locate the **Physics and Variables Selection** section. Select the **Modify model configuration for study step** checkbox.

5 In the tree, select **Component 1 (comp1)** > **Transport of Diluted Species (tds)** > **Initial Values 2**.

6 Right-click and choose **Disable**.

Step 2: Time Dependent

1 In the **Model Builder** window, 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`.

Solution 1 (sol1)

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

2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node.

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

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

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

6 In the **Store every Nth step** text field, type `10`.

The following solver settings improve and speed up the computations.

7 Right-click **Study 1 > Solver Configurations > Solution 1 (sol1) > Time-Dependent Solver 1** and choose **Fully Coupled**.

8 In the **Settings** window for **Fully Coupled**, click to expand the **Method and Termination** section.

9 From the **Nonlinear method** list, choose **Automatic (Newton)**.

Define a stop condition that terminates the computations at the lower cutoff cell voltage.

10 Right-click **Time-Dependent Solver 1** 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.liion.phis0_ec1>-V_low`	True (>=1)	√	`Stop expression 1`

14 Locate the **Output at Stop** section. From the **Add solution** list, choose **Steps before and after stop**.

15 Clear the **Add information** checkbox.

16 In the **Home** toolbar, click = **Compute**.

RESULTS

Cell Voltage and Concentration

The following steps reproduce the figures found in the documentation and fix the plot groups under the **Results** node.

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

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

3 Locate the **Plot Settings** section.

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

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

6 Select the **Two y-axes** checkbox.

7 Select the **Secondary y-axis label** checkbox. In the associated text field, type Cu⁺ concentration in cell (mol/m³).

8 Locate the **Axis** section. Select the **Manual axis limits** checkbox.

9 In the **x minimum** text field, type 3500.

10 In the **x maximum** text field, type 3750.

11 In the **y minimum** text field, type -0.25.

12 In the **y maximum** text field, type 2.

13 In the **Secondary y minimum** text field, type -10.

14 In the **Secondary y maximum** text field, type 70.

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

16 From the **Position** list, choose **Middle right**.

Global 1

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

2 In the **Settings** window for **Global**, click to expand the **Legends** section.

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

4 In the table, enter the following settings:

Legends
Deep
Shallow

Global 2

1 Right-click **Results** > **Cell Voltage and Concentration** > **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
cCu_cell	mol/m^3	Cuprous ion concentration in cell

4 Locate the **y-Axis** section. Select the **Plot on secondary y-axis** checkbox.

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

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

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

Cuprous Ion Concentration

1. In the **Model Builder** window, under **Results** click **Concentration (tds)**.
2. In the **Settings** window for **2D Plot Group**, type Cuprous Ion Concentration in the **Label** text field.
3. Click to expand the **Title** section. Locate the **Data** section. From the **Dataset** list, choose **None**.
4. Locate the **Title** section. From the **Title type** list, choose **Manual**.
5. In the **Title** text area, type Cu⁺ concentration (mol/m³).
6. Clear the **Parameter indicator** text field.
7. Locate the **Plot Settings** section. From the **View** list, choose **View 1**.
8. Click to expand the **Plot Array** section. From the **Array type** list, choose **Linear**.

Arrow Surface 1

1. In the **Model Builder** window, expand the **Cuprous Ion Concentration** node.
2. Right-click **Arrow Surface 1** and choose **Delete**.

Surface 1

1. In the **Settings** window for **Surface**, locate the **Data** section.
2. From the **Dataset** list, choose **Study 1/Parametric Solutions 1 (sol3)**.
3. From the **Parameter value (w_dent (m),depth_dent (m))** list, choose **1: w_dent=5E-4 m, depth_dent=5E-5 m**.
4. Locate the **Coloring and Style** section. From the **Color table** list, choose **Lichen**.

Line 1

1. In the **Model Builder** window, right-click **Cuprous Ion Concentration** and choose **Line**.
2. In the **Settings** window for **Line**, locate the **Data** section.
3. From the **Dataset** list, choose **Study 1/Parametric Solutions 1 (sol3)**.
4. From the **Parameter value (w_dent (m),depth_dent (m))** list, choose **1: w_dent=5E-4 m, depth_dent=5E-5 m**.
5. Locate the **Expression** section. In the **Expression** text field, type 1.
6. Locate the **Coloring and Style** section. From the **Coloring** list, choose **Uniform**.
7. From the **Color** list, choose **Black**.
8. Click to expand the **Plot Array** section. Select the **Manual indexing** checkbox.

Selection 1

1. Right-click **Line 1** and choose **Selection**.

2 Select Boundaries 3–11, 13, 14, and 16–18 only.

Annotation 1

1 In the **Model Builder** window, right-click **Cuprous Ion Concentration** and choose **Annotation**.

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

3 From the **Dataset** list, choose **Study 1/Parametric Solutions 1 (sol3)**.

4 From the **Parameter value (w_dent (m),depth_dent (m))** list, choose **1: w_dent=5E-4 m, depth_dent=5E-5 m**.

5 Locate the **Annotation** section. In the **Text** text field, type `Deep`.

6 Locate the **Coloring and Style** section. Clear the **Show point** checkbox.

7 From the **Anchor point** list, choose **Center**.

8 Click to expand the **Plot Array** section. Select the **Manual indexing** checkbox.

Annotation 1, Line 1, Surface 1

1 In the **Model Builder** window, under **Results** > **Cuprous Ion Concentration**, Ctrl-click to select **Surface 1**, **Line 1**, and **Annotation 1**.

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

Surface 2

1 In the **Settings** window for **Surface**, locate the **Data** section.

2 From the **Parameter value (w_dent (m),depth_dent (m))** list, choose **2: w_dent=0.0075 m, depth_dent=3.3333E-6 m**.

3 Click to expand the **Range** section. Locate the **Coloring and Style** section. Clear the **Color legend** checkbox.

4 Click to expand the **Inherit Style** section. From the **Plot** list, choose **Surface 1**.

5 Click to expand the **Plot Array** section. Select the **Manual indexing** checkbox.

6 In the **Index** text field, type `1`.

Line 2

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

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

3 From the **Parameter value (w_dent (m),depth_dent (m))** list, choose **2: w_dent=0.0075 m, depth_dent=3.3333E-6 m**.

4 Locate the **Plot Array** section. In the **Index** text field, type `1`.

Annotation 2

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

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

3 From the **Parameter value (w_dent (m),depth_dent (m))** list, choose **2: w_dent=0.0075 m, depth_dent=3.3333E-6 m**.

4 Locate the **Annotation** section. In the **Text** text field, type `Shallow`.

5 Locate the **Plot Array** section. In the **Index** text field, type `1`.

Deposited Copper Concentration

1 In the **Model Builder** window, right-click **Cuprous Ion Concentration** and choose **Duplicate**.

2 In the **Model Builder** window, click **Cuprous Ion Concentration 1**.

3 In the **Settings** window for **2D Plot Group**, type `Deposited Copper Concentration` in the **Label** text field.

4 Locate the **Title** section. In the **Title** text area, type `Deposited copper concentration (mol/m<sup>3</sup>)`.

Surface 1

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

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1) > Lithium-Ion Battery > Dissolving–depositing species > liion.c_pce1_CuMetal - Dissolving–depositing species concentration - mol/m³**.

3 Locate the **Coloring and Style** section. From the **Color table** list, choose **Caissara**.

Surface 2

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

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1) > Lithium-Ion Battery > Dissolving–depositing species > liion.c_pce1_CuMetal - Dissolving–depositing species concentration - mol/m³**.

3 In the **Deposited Copper Concentration** toolbar, click **Plot**.

4 Click the **Zoom Extents** button in the **Graphics** toolbar.

Electrode Potentials

1 In the **Model Builder** window, right-click **Deposited Copper Concentration** and choose **Duplicate**.

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

3 Locate the **Title** section. In the **Title** text area, type `Surface: Electrode potential (V)  Arrow Surface: Electrode current density vector`.

Surface 1

1 In the **Model Builder** window, expand the **Electrode Potentials** node, then click **Surface 1**.

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

3 From the **Time (s)** list, choose **Interpolation**.

4 In the **Time** text field, type `3604.7`.

5 Locate the **Expression** section. In the **Expression** text field, type `phis-phil`.

6 Locate the **Coloring and Style** section. From the **Color table** list, choose **MetasepiaBlue**.

Surface 2

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

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

3 From the **Time (s)** list, choose **Interpolation**.

4 In the **Time** text field, type `3604.7`.

5 Locate the **Expression** section. In the **Expression** text field, type `phis-phil`.

Arrow Surface 1

1 In the **Model Builder** window, right-click **Electrode Potentials** and choose **Arrow Surface**.

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

3 From the **Dataset** list, choose **Study 1/Parametric Solutions 1 (sol3)**.

4 From the **Parameter value (w_dent (m),depth_dent (m))** list, choose **1: w_dent=5E-4 m, depth_dent=5E-5 m**.

5 From the **Time (s)** list, choose **Interpolation**.

6 In the **Time** text field, type `3604.7`.

7 Click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)** > **Lithium-Ion Battery** > **liion.Isx,liion.Isy - Electrode current density vector**.

8 Locate the **Coloring and Style** section.

9 Select the **Scale factor** checkbox. In the associated text field, type `5e-5`.

10 From the **Color** list, choose **Black**.

11 Click to expand the **Plot Array** section. Select the **Manual indexing** checkbox.

Arrow Surface 2

1 Right-click **Arrow Surface 1** and choose **Duplicate**.

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

3 From the **Parameter value (w_dent (m),depth_dent (m))** list, choose **2: w_dent=0.0075 m, depth_dent=3.3333E-6 m**.

4 Locate the **Plot Array** section. In the **Index** text field, type `1`.

5 In the **Electrode Potentials** toolbar, click **Plot**.

6 Click the **Zoom Extents** button in the **Graphics** toolbar.

Surface 1

1 In the **Model Builder** window, under **Results** > **Cuprous Ion Concentration** click **Surface 1**.

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

3 From the **Time (s)** list, choose **Interpolation**.

4 In the **Time** text field, type `3604.7`.

Surface 2

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

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

3 From the **Time (s)** list, choose **Interpolation**.

4 In the **Time** text field, type `3604.7`.

5 In the **Cuprous Ion Concentration** toolbar, click **Plot**.

6 Click the **Zoom Extents** button in the **Graphics** toolbar.

Electrolyte Salt Concentration

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

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

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

4 Locate the **Title** section. In the **Title** text area, type `Surface: c<sub>l</sub> concentration (mol/m<sup>3</sup>) Arrow Surface: Electrolyte current density vector`.

Surface 1

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

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

3 From the **Time (s)** list, choose **Last (3749.3)**.

4 Locate the **Expression** section. In the **Expression** text field, type `cl-cCu`.

5 Locate the **Coloring and Style** section. From the **Color table** list, choose **Prionace**.

Surface 2

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

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

3 From the **Time (s)** list, choose **Last (3726)**.

4 Locate the **Expression** section. In the **Expression** text field, type `cl-cCu`.

Arrow Surface 1

1 In the **Model Builder** window, click **Arrow Surface 1**.

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

3 From the **Time (s)** list, choose **Last (3749.3)**.

4 Click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)** > **Lithium-Ion Battery** > **liion.Ilx,liion.Ily - Electrolyte current density vector**.

5 Locate the **Coloring and Style** section. From the **Color** list, choose **Cyan**.

Arrow Surface 2

1 In the **Model Builder** window, click **Arrow Surface 2**.

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

3 From the **Time (s)** list, choose **Last (3726)**.

4 Click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)** > **Lithium-Ion Battery** > **liion.Ilx,liion.Ily - Electrolyte current density vector**.

5 Locate the **Coloring and Style** section. From the **Color** list, choose **Cyan**.

Current Collector Dissolution Current

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

2 In the **Settings** window for **1D Plot Group**, type `Current Collector Dissolution Current` in the **Label** text field.

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

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

Line Graph 1

1 Right-click **Current Collector Dissolution Current** and choose **Line Graph**.

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

3. From the **Dataset** list, choose **Study 1/Parametric Solutions 1 (sol3)**.
4. From the **Parameter selection (w_dent, depth_dent)** list, choose **First**.
5. From the **Time selection** list, choose **Interpolated**.
6. In the **Times (s)** text field, type `3604.7`.
7. Select Boundary 4 only.
8. Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)** > **Lithium-Ion Battery** > **Electrode kinetics** > **liion.iloc_er1 - Local current density - A/m^2**.
9. Click to expand the **Legends** section. Select the **Show legends** checkbox.
10. From the **Legends** list, choose **Manual**.
11. In the table, enter the following settings:

Legends
`Deep, local E<sub>neg</sub> >3.5 V`

Line Graph 2

1. Right-click **Line Graph 1** and choose **Duplicate**.
2. In the **Settings** window for **Line Graph**, locate the **Data** section.
3. From the **Time selection** list, choose **Last**.
4. Locate the **Legends** section. In the table, enter the following settings:

Legends
`Deep, E<sub>cell</sub>=-0.05 V`

Line Graph 1, Line Graph 2

1. In the **Model Builder** window, under **Results** > **Current Collector Dissolution Current**, Ctrl-click to select **Line Graph 1** and **Line Graph 2**.
2. Right-click and choose **Duplicate**.

Line Graph 3

1. In the **Settings** window for **Line Graph**, locate the **Data** section.
2. From the **Parameter selection (w_dent, depth_dent)** list, choose **Last**.
3. Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.

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

Legends
Shallow, local E_{neg} >3.5 V

Line Graph 4

1 In the **Model Builder** window, click **Line Graph 4**.

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

3 From the **Parameter selection (w_dent, depth_dent)** list, choose **Last**.

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

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

Legends
Shallow, E_{cell}=-0.05 V

6 In the **Current Collector Dissolution Current** toolbar, click **Plot**.

Finally, remove redundant plots.

Average Electrode State of Charge (liion), Electrode Potential with Respect to Adjacent Reference (liion), Electrode Potential with Respect to Ground (liion), Electrolyte Salt Concentration (liion), Particle Surface State of Charge (liion), Separator Current Density Magnitude (liion)

1 In the **Model Builder** window, under **Results**, Ctrl-click to select **Average Electrode State of Charge (liion)**, **Electrode Potential with Respect to Ground (liion)**, **Electrode Potential with Respect to Adjacent Reference (liion)**, **Electrolyte Salt Concentration (liion)**, **Separator Current Density Magnitude (liion)**, and **Particle Surface State of Charge (liion)**.

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

Cuprous Ion Concentration

Click the **Zoom Extents** button in the **Graphics** toolbar.