Edge Effects in a Spirally Wound Lithium-Ion Battery

Introduction

Due to the large differences in length scales in a lithium-ion battery, with the thickness of the different layers typically being several orders of magnitude smaller than the extension in the sheet direction, a lithium-ion battery is often well represented by a one-dimensional model. However, the packing and stacking of the battery may cause edge effects which motivate modeling in higher dimensions.

This example investigates the geometrical effects that occur when a constructing a lithium-ion battery by spirally winding the active battery components to construct a cylindrical "jelly-roll" battery.

Model Definition

The battery is constructed by winding a laminated bi-battery sheet into a spiral, which is placed in a cylinder and filled with liquid electrolyte. The battery model consists of the following parts (See Figure 1):

- Two negative porous electrodes (60 µm thick)
- Two positive porous electrodes (60 µm thick)
- One negative current collector (14 µm thick)
- One positive current collector (20 µm thick)
- Two separator regions (30 µm thick)
- One inner and one outer liquid electrolyte region, filling up the hollow space between the active components and the circular battery casing

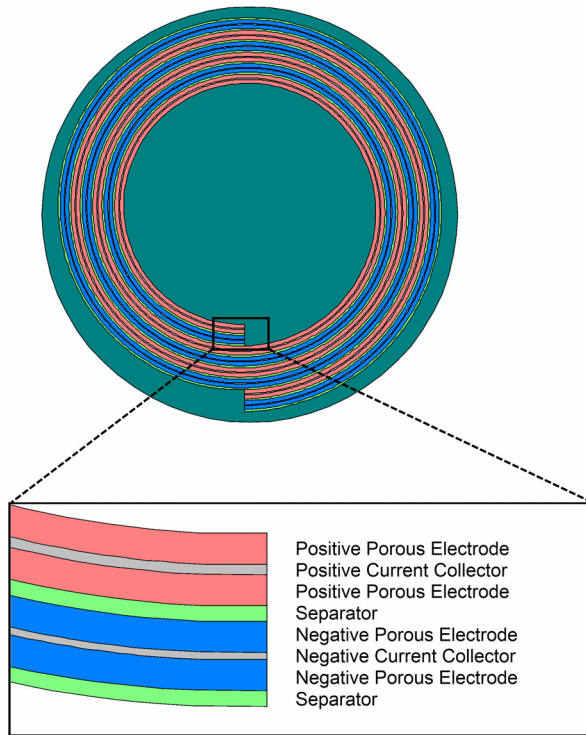The spiral revolves three full laps.

Figure 1: Modeled geometry. Spirally wound bi-battery in circular casing filled with liquid electrolyte.

The Lithium-Ion Battery interface is used to model the battery. For a detailed model description, see the accompanying example 1D Isothermal Lithium-Ion Battery found in the Battery Design Module Application Libraries.

The negative current collector at the outer end of the spiral is grounded, and a current density condition is applied to the end of the positive current collector at the inner end of the spiral.

The load cycle investigated is a constant discharge of the battery to approximately 50% state-of-charge. Two different constant discharge rates are compared, 1C and 10C, where 1C corresponds to the discharge current needed for a 100% discharges in one hour, and

10C a ten times higher discharge current. A 10,000 second relaxation simulation after the 1C discharge is also performed.

Results and Discussion

Figure 2 shows the cell potential versus time during the 1C discharge.
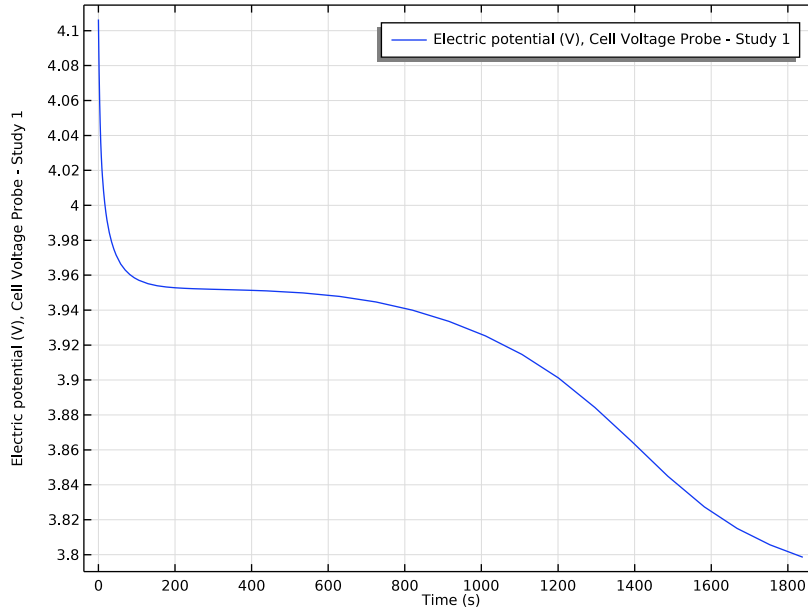

Figure 2: Cell potential versus time during the 1C discharge.

Figure 3 and Figure 4 show the relative lithium concentration at the surface of the electrode particles for the negative and positive porous electrode regions at the end of the 1C discharge (t = 1800 s). Due to the resulting large electrolyte resistivity for lithium transport from and to the innermost and outermost parts of the spiral, these areas of the porous electrodes are hardly discharged at all.

The discharge rate is higher for the negative electrode at the inner end of the spiral and at the outer end for the positive electrodes. This is an effect of the outermost or innermost porous electrode regions contributing to the electrochemical current close to the spiral ends.

These locally higher discharge rates at the ends typically results in a shorter lifetime for these regions than for the inner parts of the spiral, which are discharged more uniformly.

However, for a battery with more windings, the relative area of these end regions is small compared to the inner part of the spiral.
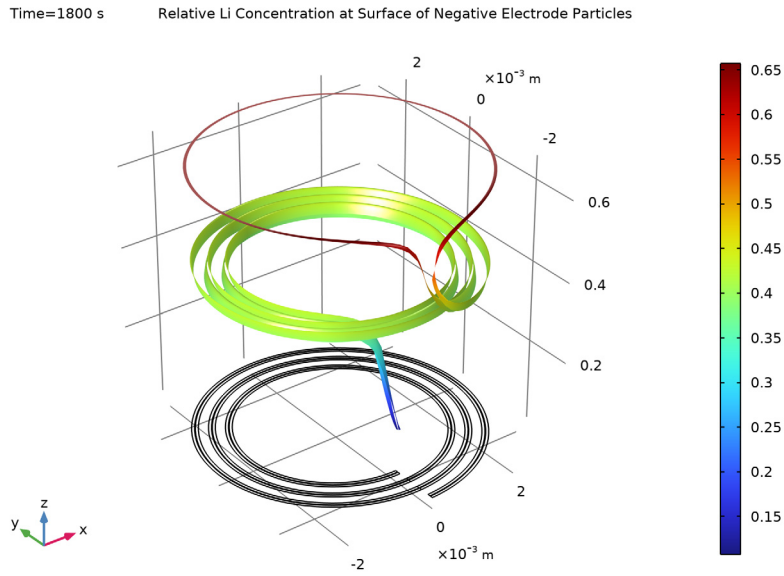

Figure 3: Relative lithium concentration at the surface of the negative electrode particles during at t = 1800 s for the 1C discharge.

For this system, there is an excess of negative porous electrode material, and therefore the negative electrode does not get fully depleted in areas where the positive electrode reaches lithium saturation (a relative lithium concentration close to unity in relation to the maximum possible concentration).
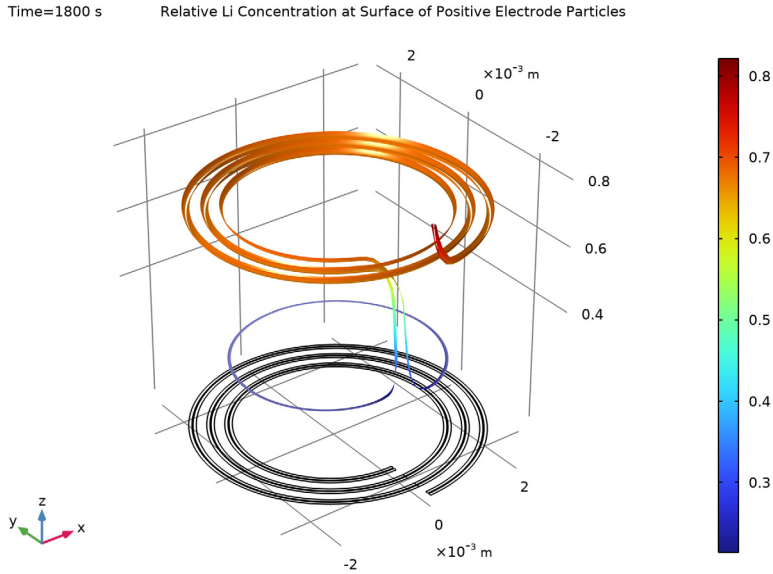
Time=1800 s   Relative Li Concentration at Surface of Positive Electrode Particles

Figure 4: Relative lithium concentration at the surface of the positive electrode particles during at t = 1800 s for the 1C discharge.

Figure 5 shows the electrolyte potential at the end of the 1C discharge cycle (t = 1800 s). There is a significant drop in potential from the outer liquid electrolyte region through the spiral into the inner electrolyte region. This is an effect of the outermost and innermost porous electrode regions being discharged at a much lower rate than the rest of the system due to large ohmic drops in the electrolyte, and thereby in effect having almost constant equilibrium potentials throughout the discharge. The potential gradients indicate that there is a current flowing also in the spiral direction close to the spiral ends.
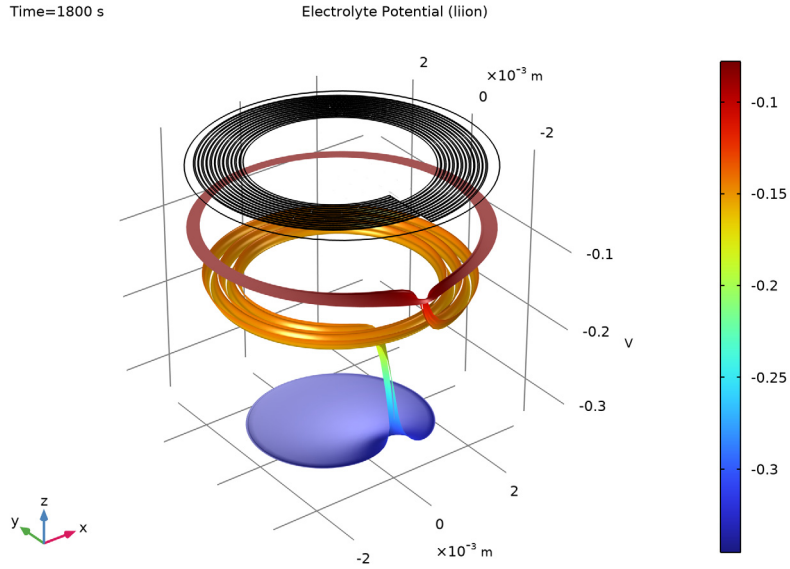
Figure 5: Electrolyte potential at t = 1800 s for the 1C discharge.

Figure 6 shows the electrolyte salt concentration at the end of the 1C discharge (t = 1800 s). The concentration gradients close to the spiral ends are due to the current flowing in the spiral direction.
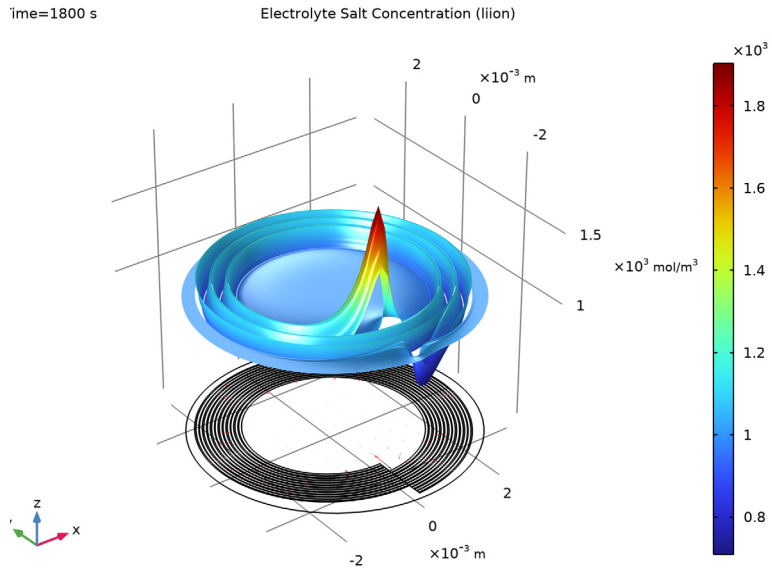
Electrolyte Salt Concentration (liion)

Figure 6: Electrolyte salt concentration at t = 1800 s for the 1C discharge.

The plots for the 10C discharge of cell voltage versus time, lithium concentrations, the electrolyte potential, and electrolyte salt concentration and lithium concentrations are shown in Figure 7 to Figure 11.

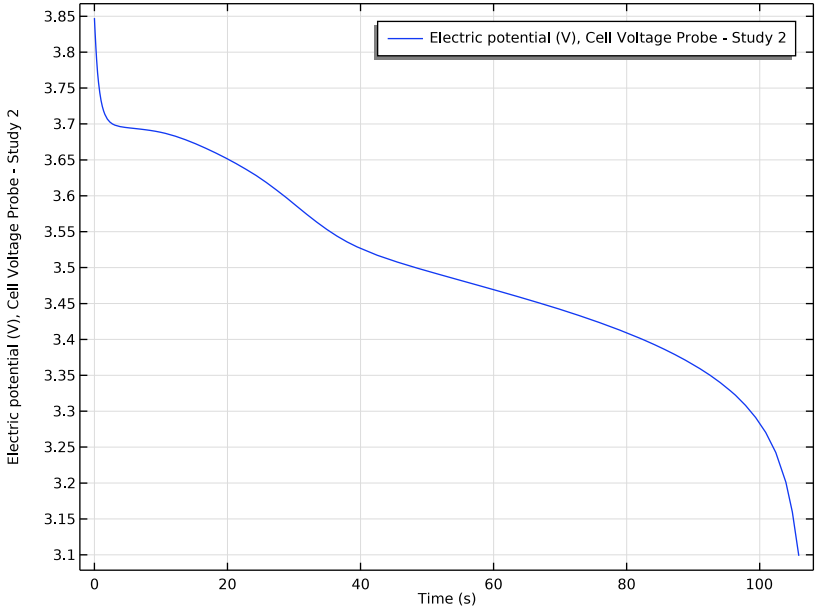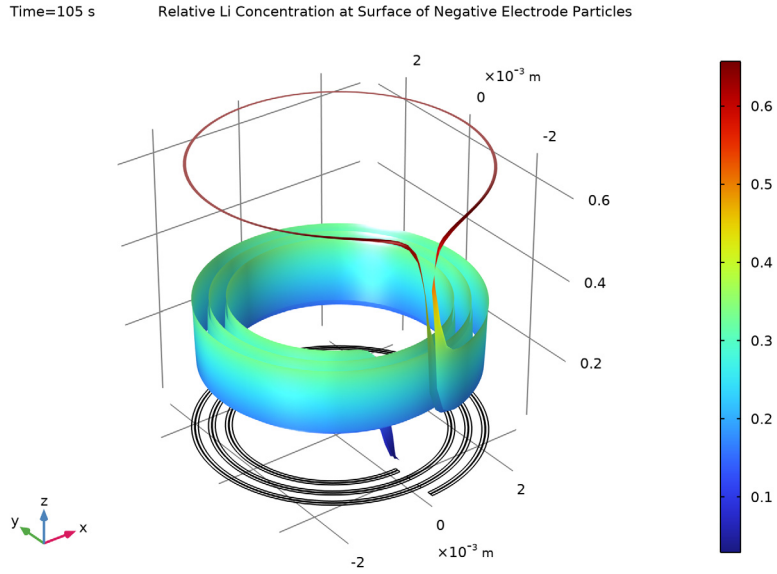*Figure 7: Cell potential versus time during the 10C discharge.*

Time=105 s   Relative Li Concentration at Surface of Negative Electrode Particles

Figure 8: Relative lithium concentration at the surface of the negative electrode particles
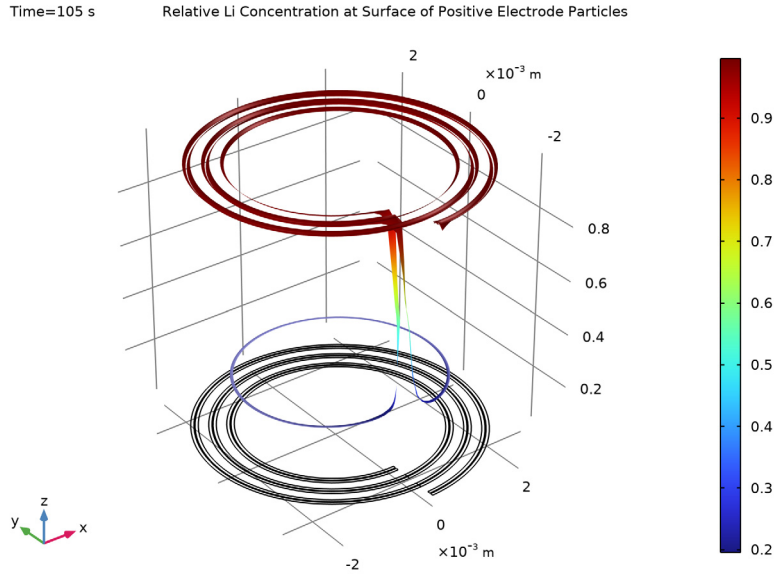
during at t = 180 s for the 10C discharge.

Time=105 s   Relative Li Concentration at Surface of Positive Electrode Particles

Figure 9: Relative lithium concentration at the surface of the positive electrode particles during at t = 180 s for the 10C discharge.

The higher discharge rates result in higher gradients in the battery direction compared to the spiral direction, giving less pronounced edge effects and a more uniform discharge.
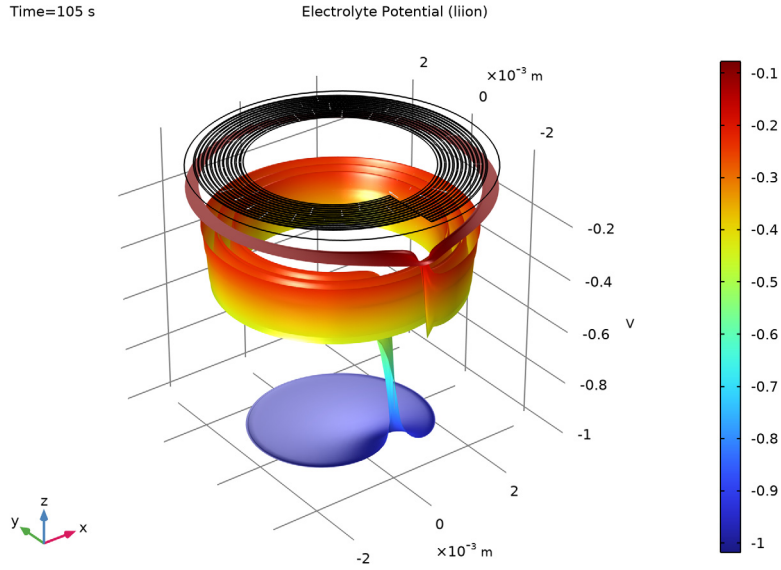
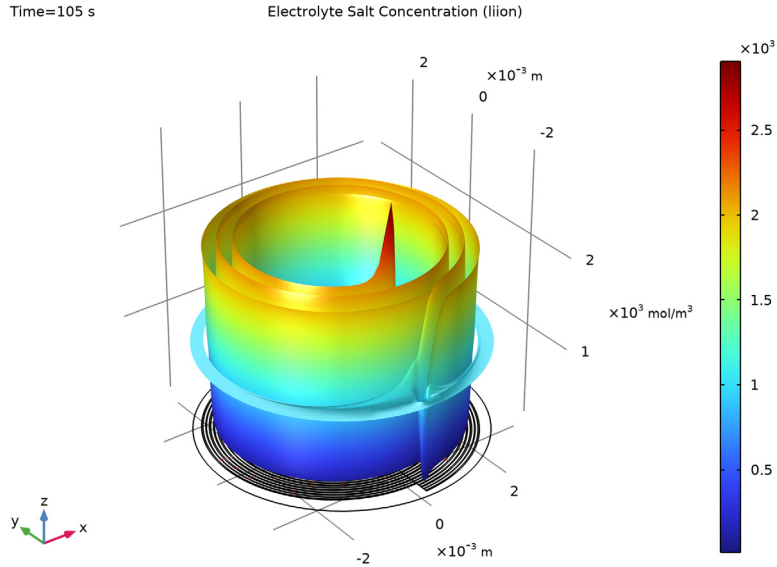*Figure 10: Electrolyte potential at t = 180 s for the 10C discharge.*

Figure 11: Electrolyte salt concentration at t = 180 s for the 10C discharge.

Figure 12 to Figure 16 depict the cell potential, lithium concentrations, electrolyte potential, and electrolyte salt concentration at the end of a **10,000** s relaxation simulation after the 50% discharge at 1C. After approx **3** h of relaxation the battery has not yet reached complete equilibrium.

The first steep rise in cell voltage (Figure 12) is closely related to the same relaxation phenomenon seen in the 1D Isothermal Lithium-Ion Battery model, whereas the slower rise after the first minutes is attributed to moving lithium to and from the outermost and innermost part of the spiral, a process that is very slow due to the long traveling distance in the spiral direction.
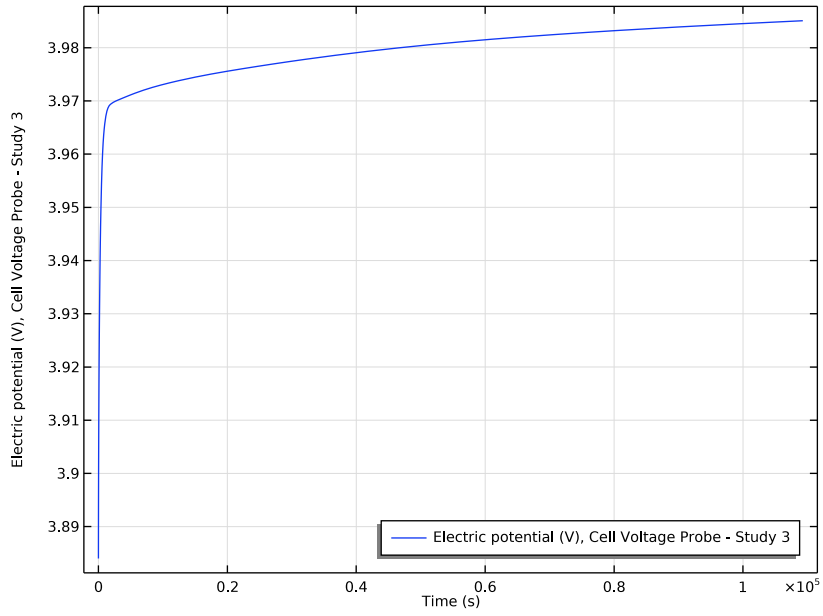
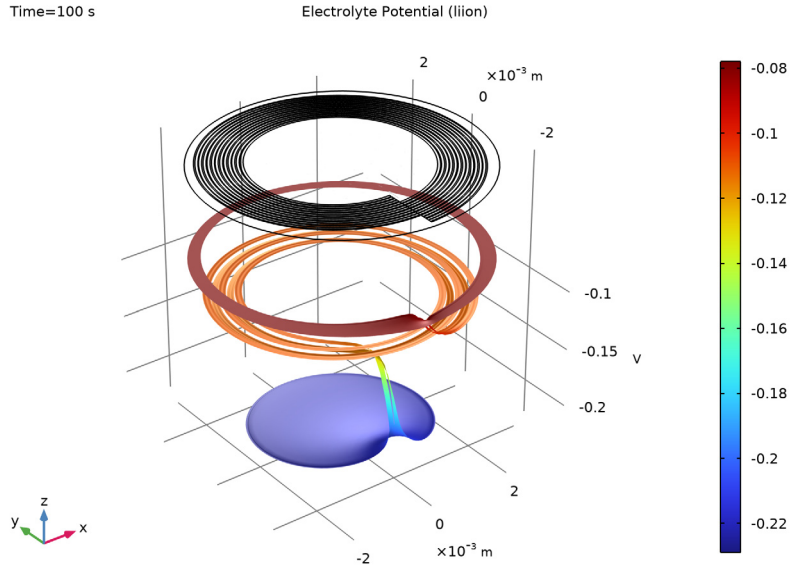*Figure 12: Cell potential versus time during the relaxation simulation.*

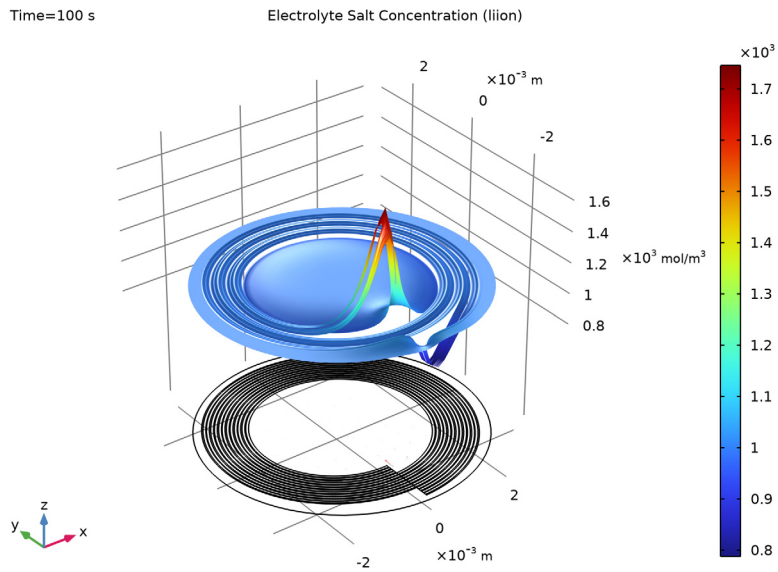*Figure 13: Electrolyte potential at t = 10,000 s for the relaxation simulation.*

Figure 14: Electrolyte salt concentration at t = 10,000 s for the relaxation simulation.

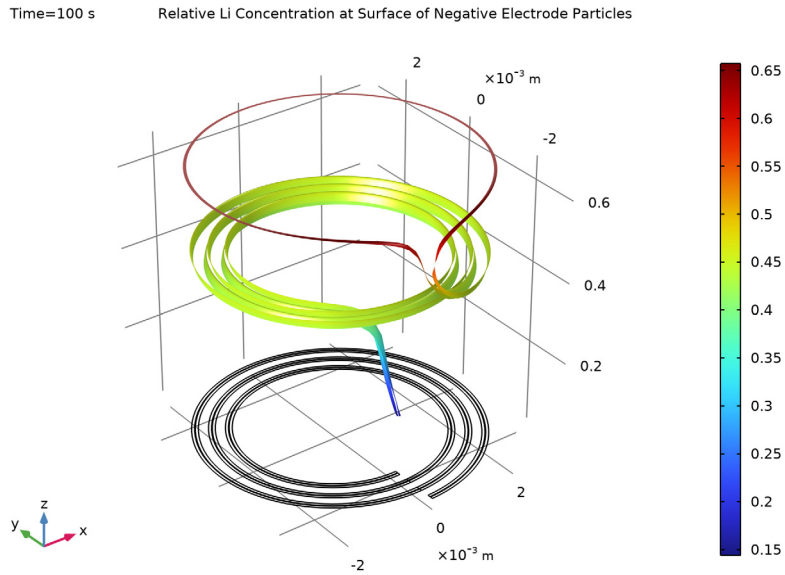Time=100 s   Relative Li Concentration at Surface of Negative Electrode Particles

Figure 15: Relative lithium concentration at the surface of the negative electrode particles during at t = 10,000 s for the relaxation simulation.

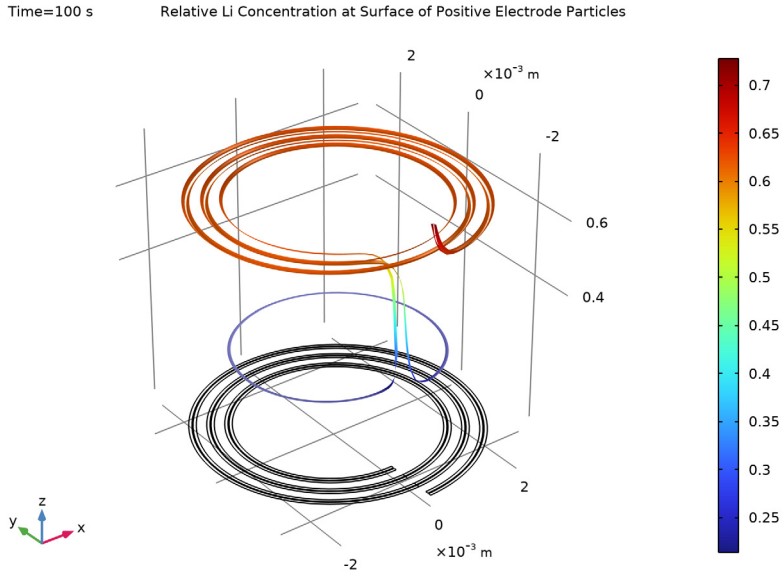Time=100 s   Relative Li Concentration at Surface of Positive Electrode Particles

Figure 16: Relative lithium concentration at the surface of the positive electrode particles during at t = 10,000 s for the relaxation simulation.

Notes About the COMSOL Implementation

To minimize the computation time, the element order has been decreased to 1 for the potentials and the electrolyte concentration variables, and a quite coarse mapped mesh is used. 1D battery simulations were made in order to check that the accuracy of the results were not significantly compromised when minimizing the computational degrees of freedom in this way.

Reference

1. M. Doyle, J. Newman, A.S. Gozdz, C.N. Schmutz, and J.M. Tarascon, "Comparison of Modeling Predictions with Experimental Data from Plastic Lithium Ion Cells," *J. Electrochem. Soc.*, vol. 143, no. 6, pp. 1890–1903, 1996.

Application Library path: `Battery_Design_Module/Batteries,_Lithium-Ion/ li_battery_spiral_2d`

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 Click ➜ **Study**.

5 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces> Time Dependent with Initialization**.

6 Click ☑ **Done**.

GLOBAL DEFINITIONS

Parameters 1

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

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

3 Click 📂 **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `li_battery_spiral_2d_parameters.txt`.

Analytic 1 (an1)

Add the following functions to be used when drawing the spiral.

1 In the **Home** toolbar, click f(x) **Functions** and choose **Global>Analytic**.

2 In the **Settings** window for **Analytic**, type `spiralX` in the **Function name** text field.

3 Locate the **Definition** section. In the **Expression** text field, type `-(s/(2*pi)*D_tot+R)* sin(s)`.

4 In the **Arguments** text field, type s, R.

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

Argument	Unit
s	1
R	m

6 In the **Function** text field, type m.

Analytic 2 (spiralX2)

1 Right-click **Analytic 1 (an1)** and choose **Duplicate**.

2 In the **Settings** window for **Analytic**, type spiralY in the **Function name** text field.

3 Locate the **Definition** section. In the **Expression** text field, type -(s/(2*pi)*D_tot+R)*cos(s).

GEOMETRY 1

Now draw the spiral, consisting of eight different layers.

Parametric Curve 1 (pc1)

1 In the **Geometry** toolbar, click **More Primitives** and choose **Parametric Curve**.

2 In the **Settings** window for **Parametric Curve**, locate the **Parameter** section.

3 In the **Maximum** text field, type w_tot+2*pi.

4 Locate the **Expressions** section. In the **x** text field, type spiralX(s,r0).

5 In the **y** text field, type spiralY(s,r0).

6 Click **Build Selected**.

Parametric Curve 2 (pc2)

1 Right-click **Parametric Curve 1 (pc1)** and choose **Duplicate**.

2 In the **Settings** window for **Parametric Curve**, locate the **Expressions** section.

3 In the **x** text field, type spiralX(s,r0+a1).

4 In the **y** text field, type spiralY(s,r0+a1).

5 Click **Build Selected**.

Parametric Curve 3 (pc3)

1 Right-click **Parametric Curve 2 (pc2)** and choose **Duplicate**.

2 In the **Settings** window for **Parametric Curve**, locate the **Expressions** section.

3 In the **x** text field, type spiralX(s,r0+a1+a2).

4 In the **y** text field, type `spiralY(s,r0+a1+a2)`.

5 Click 🔳 **Build Selected**.

Parametric Curve 4 (pc4)

1 Right-click **Parametric Curve 3 (pc3)** and choose **Duplicate**.

2 In the **Settings** window for **Parametric Curve**, locate the **Expressions** section.

3 In the **x** text field, type `spiralX(s,r0+a1+a2+a3)`.

4 In the **y** text field, type `spiralY(s,r0+a1+a2+a3)`.

5 Click 🔳 **Build Selected**.

Parametric Curve 5 (pc5)

1 Right-click **Parametric Curve 4 (pc4)** and choose **Duplicate**.

2 In the **Settings** window for **Parametric Curve**, locate the **Expressions** section.

3 In the **x** text field, type `spiralX(s,r0+a1+a2+a3+a4)`.

4 In the **y** text field, type `spiralY(s,r0+a1+a2+a3+a4)`.

5 Click 🔳 **Build Selected**.

Parametric Curve 6 (pc6)

1 Right-click **Parametric Curve 5 (pc5)** and choose **Duplicate**.

2 In the **Settings** window for **Parametric Curve**, locate the **Expressions** section.

3 In the **x** text field, type `spiralX(s,r0+a1+a2+a3+a4+a5)`.

4 In the **y** text field, type `spiralY(s,r0+a1+a2+a3+a4+a5)`.

5 Click 🔳 **Build Selected**.

Parametric Curve 7 (pc7)

1 Right-click **Parametric Curve 6 (pc6)** and choose **Duplicate**.

2 In the **Settings** window for **Parametric Curve**, locate the **Expressions** section.

3 In the **x** text field, type `spiralX(s,r0+a1+a2+a3+a4+a5+a6)`.

4 In the **y** text field, type `spiralY(s,r0+a1+a2+a3+a4+a5+a6)`.

5 Click 🔳 **Build Selected**.

Parametric Curve 8 (pc8)

1 Right-click **Parametric Curve 7 (pc7)** and choose **Duplicate**.

2 In the **Settings** window for **Parametric Curve**, locate the **Expressions** section.

3 In the **x** text field, type `spiralX(s,r0+a1+a2+a3+a4+a5+a6+a7)`.

4 In the **y** text field, type `spiralY(s,r0+a1+a2+a3+a4+a5+a6+a7)`.

5 Click ⬛ **Build Selected**.

Parametric Curve 9 (pc9)
1 In the **Geometry** toolbar, click ⚡ **More Primitives** and choose **Parametric Curve**.

2 In the **Settings** window for **Parametric Curve**, locate the **Parameter** section.

3 In the **Maximum** text field, type D_tot*(laps+1).

4 Locate the **Expressions** section. In the **x** text field, type 0.

5 In the **y** text field, type -(s+r0).

6 Click ⬛ **Build Selected**.

Convert to Solid 1 (csol1)
1 In the **Geometry** toolbar, click 🔲 **Conversions** and choose **Convert to Solid**.

2 Click in the **Graphics** window and then press Ctrl+A to select all objects.

3 In the **Settings** window for **Convert to Solid**, click ⬛ **Build Selected**.

Circle 1 (c1)
1 In the **Geometry** toolbar, click ⊙ **Circle**.

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

3 In the **Radius** text field, type D_tot*(laps+1.25)+r0.

4 Locate the **Position** section. In the **x** text field, type D_tot/4.

5 In the **y** text field, type -D_tot/4.

6 Click ⬛ **Build All Objects**.

DEFINITIONS

Next, make selections of the various domains to use later on when setting up the physics.

Positive current collector
1 In the **Definitions** toolbar, click 🗂 **Explicit**.

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

3 Select Domains 8, 16, and 24 only.

Negative current collector
1 In the **Definitions** toolbar, click 🗂 **Explicit**.

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

3 Select Domains 4, 12, and 20 only.

Positive porous electrode

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

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

3 Select Domains 7, 9, 15, 17, 23, and 25 only.

Negative porous electrode

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

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

3 Select Domains 3, 5, 11, 13, 19, and 21 only.

Electrolyte

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

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

3 Select Domains 2, 6, 10, 14, 18, and 22 only.

Negative terminal

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

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

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

4 Select Boundary 9 only.

Positive terminal

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

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

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

4 Select Boundary 60 only.

Electrolyte outside

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

2 In the **Settings** window for **Explicit**, type Electrolyte outside in the **Label** text field.

3 Select Domains 1 and 26 only.

Spiral battery

1 In the **Definitions** toolbar, click 🗔 **Union**.

2 In the **Settings** window for **Union**, type Spiral battery in the **Label** text field.

3 Locate the **Input Entities** section. Under **Selections to add**, click ╋ **Add**.

4 In the **Add** dialog box, in the **Selections to add** list, choose **Positive current collector**, **Negative current collector**, **Positive porous electrode**, **Negative porous electrode**, and **Electrolyte**.

5 Click **OK**.

Positive + Electrolyte + Negative

1 In the **Definitions** toolbar, click ⊞ **Union**.

2 In the **Settings** window for **Union**, type `Positive + Electrolyte + Negative` in the **Label** text field.

3 Locate the **Input Entities** section. Under **Selections to add**, click ╋ **Add**.

4 In the **Add** dialog box, in the **Selections to add** list, choose **Positive porous electrode**, **Negative porous electrode**, **Electrolyte**, and **Electrolyte outside**.

5 Click **OK**.

MATERIALS

Use data from the material library for the current collector materials.

ADD MATERIAL

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

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

3 In the tree, select **Built-in>Aluminum**.

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

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

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

MATERIALS

Aluminum (mat1)

1 In the **Model Builder** window, under **Component 1 (comp1)>Materials** click **Aluminum (mat1)**.

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

3 From the **Selection** list, choose **Positive current collector**.

Copper (mat2)

1 In the **Model Builder** window, click **Copper (mat2)**.

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

3 From the **Selection** list, choose **Negative current collector**.

ADD MATERIAL

Use the Battery Material Library to set up the material properties for the electrolyte and electrode materials. By adding the electrolyte material to the model first, this material becomes the default material for all domains.

Note: In the Materials node, `cEeqref` denotes the maximum lithium concentration in the active material.

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

2 In the tree, select **Battery>Electrolytes>LiPF6 in 1:2 EC:DMC and p(VdF-HFP) (Polymer, Li-ion Battery)**.

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

4 In the tree, select **Battery>Electrodes>Graphite, LixC6 MCMB (Negative, Li-ion Battery)**.

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

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

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

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

MATERIALS

LiPF6 in 1:2 EC:DMC and p(VdF-HFP) (Polymer, Li-ion Battery) (mat3)

1 In the **Model Builder** window, under **Component 1 (comp1)>Materials** click **LiPF6 in 1:2 EC:DMC and p(VdF-HFP) (Polymer, Li-ion Battery) (mat3)**.

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

3 From the **Selection** list, choose **Positive + Electrolyte + Negative**.

LITHIUM-ION BATTERY (LIION)

Now start defining the battery physics model.

Porous Electrode 1

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

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

3 From the **Selection** list, choose **Negative porous electrode**.

4 Locate the **Electrode Properties** section. From the **Electrode material** list, choose **Graphite, LixC6 MCMB (Negative, Li-ion Battery) (mat4)**.

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

6 In the ε_l text field, type epsl_neg.

Particle Intercalation 1

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

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

3 From the **Particle material** list, choose **Graphite, LixC6 MCMB (Negative, Li-ion Battery) (mat4)**.

4 Locate the **Species Settings** section. In the $c_{s,init}$ text field, type cs0_neg.

5 Locate the **Particle Transport Properties** section. In the r_p text field, type rp_neg.

6 Click to expand the **Particle Discretization** section. In the N_{el} text field, type 3.

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 **Material** section.

3 From the **Material** list, choose **Graphite, LixC6 MCMB (Negative, Li-ion Battery) (mat4)**.

4 Locate the **Electrode Kinetics** section. In the $i_{0,ref}(T)$ text field, type i0ref_neg.

5 In the α_a text field, type aA_neg.

6 In the α_c text field, type aC_neg.

Porous Electrode 2

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

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

3 From the **Selection** list, choose **Positive porous electrode**.

4 Locate the **Electrode Properties** section. From the **Electrode material** list, choose **LMO, LiMn2O4 Spinel (Positive, Li-ion Battery) (mat5)**.

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

6 In the ε_l text field, type epsl_pos.

Particle Intercalation 1

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

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

3 From the **Particle material** list, choose **LMO, LiMn2O4 Spinel (Positive, Li-ion Battery) (mat5)**.

4 Locate the **Species Settings** section. In the $c_{s,init}$ text field, type cs0_pos.

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

6 Locate the **Particle Discretization** section. In the N_{el} text field, type 5.

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 **Material** section.

3 From the **Material** list, choose **LMO, LiMn2O4 Spinel (Positive, Li-ion Battery) (mat5)**.

4 Locate the **Electrode Kinetics** section. In the $i_{0,\mathrm{ref}}(T)$ text field, type i0ref_pos.

5 In the α_a text field, type aA_pos.

6 In the α_c text field, type aC_pos.

Electrode 1

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

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

3 From the **Selection** list, choose **Negative current collector**.

Electrode 2

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

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

3 From the **Selection** list, choose **Positive current collector**.

Electric Ground 1

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

2 In the **Settings** window for **Electric Ground**, locate the **Boundary Selection** section.

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

Electrode Current Density - 1C Discharge

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

This node will be used in the 1C discharge study.

2 In the **Settings** window for **Electrode Current Density**, type Electrode Current Density - 1C Discharge in the **Label** text field.

3 Locate the **Boundary Selection** section. From the **Selection** list, choose **Positive terminal**.

4 Locate the **Electrode Current Density** section. In the $i_{n,\mathrm{s}}$ text field, type i_app_1C.

Electrode Current Density - 10C Discharge

Create a second electrode current density node to be used for the 10 C discharge study

1 Right-click **Electrode Current Density - 1C Discharge** and choose **Duplicate**.

2 In the **Settings** window for **Electrode Current Density**, type Electrode Current Density - 10C Discharge in the **Label** text field.

3 Locate the **Electrode Current Density** section. In the $i_{n,\mathrm{s}}$ text field, type 10*i_app_1C.

Set the element order to one for the potentials and the electrolyte concentration variables in the battery model to reduce the computation time.

4 In the **Model Builder** window, click **Lithium-Ion Battery (liion)**.

5 In the **Settings** window for **Lithium-Ion Battery**, click to expand the **Discretization** section.

6 From the **Electrolyte potential** list, choose **Linear**.

7 From the **Electrolyte salt concentration** list, choose **Linear**.

8 From the **Electric potential** list, choose **Linear**.

MESH 1

Now start building the mesh. In the spiral direction you can expect low gradients. Use a mapped mesh to reflect this and to optimize the number of elements.

Edge 1

1 In the **Mesh** toolbar, click △ **Edge**.

2 Select Boundaries 9 and 17 only.

Distribution 1

1 Right-click **Edge 1** and choose **Distribution**.

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

3 In the **Number of elements** text field, type 1.

Edge 2

1 In the **Mesh** toolbar, click △ **Edge**.

2 Select Boundaries 5 and 13 only.

Distribution 1

1 Right-click **Edge 2** and choose **Distribution**.

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

3 In the **Number of elements** text field, type 4.

Edge 3

1 In the **Mesh** toolbar, click △ **Edge**.

2 Select Boundaries 11 and 19 only.

Distribution 1

1 Right-click **Edge 3** and choose **Distribution**.

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

3 In the **Number of elements** text field, type 10.

Edge 4

1 In the **Mesh** toolbar, click ⬛ **Edge**.

2 Select Boundaries 7 and 15 only.

Distribution 1

1 Right-click **Edge 4** and choose **Distribution**.

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

3 In the **Number of elements** text field, type 6.

Edge 5

1 In the **Mesh** toolbar, click ⬛ **Edge**.

2 Select Boundaries 6, 8, 10, 12, 14, 16, 18, 20, 22, 24, 26, 28, 30, 32, 34, 36, 38, 40, 42, 44, 46, 48, 50, 52, and 54 only.

Distribution 1

1 Right-click **Edge 5** and choose **Distribution**.

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

3 From the **Distribution type** list, choose **Explicit**.

4 In the **Relative placement of vertices along edge** text field, type 0 5e-5 10^range(-4, 0.25,-2) range(2e-2,1e-2,0.98) (1-10^range(-2,-0.25,-4)) 0.99995 1.

Mapped 1

1 In the **Mesh** toolbar, click ⬛ **Mapped**.

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

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

4 From the **Selection** list, choose **Spiral battery**.

Free Triangular 1

1 In the **Mesh** toolbar, click ⬛ **Free Triangular**.

2 In the **Model Builder** window, right-click **Mesh 1** and choose **Build All**.

DEFINITIONS (COMP1)

Add a probe to store the average potential of the positive terminal for all solver time steps.

Cell Voltage Probe - Study 1

1 In the **Definitions** toolbar, click 🖊 **Probes** and choose **Boundary Probe**.

2 In the **Settings** window for **Boundary Probe**, type Cell Voltage Probe - Study 1 in the **Label** text field.

3 Locate the **Source Selection** section. From the **Selection** list, choose **Positive terminal**.

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

STUDY 1

Step 2: Time Dependent

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

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

3 In the **Output times** text field, type range(0,300,1800).

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

5 In the tree, select **Component 1 (Comp1)>Lithium-Ion Battery (Liion)> Electrode Current Density - 10C Discharge**.

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

7 In the **Model Builder** window, click **Study 1**.

8 In the **Settings** window for **Study**, type Study 1 - 1 C Discharge in the **Label** text field.

9 In the **Home** toolbar, click ▬ **Compute**.

RESULTS

Electrolyte Salt Concentration (liion)

1 In the **Model Builder** window, under **Results** click **Electrolyte Salt Concentration (liion)**.

2 In the **Settings** window for **2D Plot Group**, click to expand the **Title** section.

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

Height Expression 1

1 In the **Model Builder** window, expand the **Electrolyte Salt Concentration (liion)** node.

2 Right-click **Surface 1** and choose **Height Expression**.

3 In the **Electrolyte Salt Concentration (liion)** toolbar, click 🔲 **Plot**.

Electrolyte Potential (liion)

1 In the **Model Builder** window, under **Results** click **Electrolyte Potential (liion)**.

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

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

Height Expression 1

1 In the **Model Builder** window, expand the **Electrolyte Potential (liion)** node.

2 Right-click **Surface 1** and choose **Height Expression**.

3 In the **Electrolyte Potential (liion)** toolbar, click ⊡ **Plot**.

Cell Voltage - Study 1

1 In the **Model Builder** window, under **Results** click **Probe Plot Group 7**.

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

3 In the **Cell Voltage - Study 1** toolbar, click ⊡ **Plot**.

Study 1 - 1 C Discharge/Solution 1 (4) (sol1)

In the **Results** toolbar, click ▦ **More Datasets** and choose **Solution**.

Selection

1 In the **Results** toolbar, click ⧉ **Attributes** and choose **Selection**.

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

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

4 From the **Selection** list, choose **Negative porous electrode**.

Study 1 - 1 C Discharge/Solution 1 (5) (sol1)

In the **Results** toolbar, click ▦ **More Datasets** and choose **Solution**.

Selection

1 In the **Results** toolbar, click ⧉ **Attributes** and choose **Selection**.

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

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

4 From the **Selection** list, choose **Positive porous electrode**.

Relative Li Concentration at Surface of Negative Electrode Particles

1 In the **Results** toolbar, click ▪ **2D Plot Group**.

2 In the **Settings** window for **2D Plot Group**, type Relative Li Concentration at Surface of Negative Electrode Particles in the **Label** text field.

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

4 Locate the **Data** section. From the **Dataset** list, choose **Study 1 - 1 C Discharge/ Solution 1 (4) (sol1)**.

Surface 1

1 Right-click **Relative Li Concentration at Surface of Negative Electrode Particles** and choose **Surface**.

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>Particle intercalation>liion.socloc_surface - Local electrode material state-of-charge, particle surface**.

Height Expression 1

1 Right-click **Surface 1** and choose **Height Expression**.

2 In the **Relative Li Concentration at Surface of Negative Electrode Particles** toolbar, click ▣ **Plot**.

Relative Li Concentration at Surface of Positive Electrode Particles

1 In the **Home** toolbar, click ▣ **Add Plot Group** and choose **2D Plot Group**.

2 In the **Settings** window for **2D Plot Group**, type Relative Li Concentration at Surface of Positive Electrode Particles in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1 - 1 C Discharge/ Solution 1 (5) (sol1)**.

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

Surface 1

1 Right-click **Relative Li Concentration at Surface of Positive Electrode Particles** and choose **Surface**.

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>Particle intercalation>liion.socloc_surface - Local electrode material state-of-charge, particle surface**.

Height Expression 1

1 Right-click **Surface 1** and choose **Height Expression**.

2 In the **Relative Li Concentration at Surface of Positive Electrode Particles** toolbar, click ▣ **Plot**.

ROOT

Now, perform a new simulation for a 10 C discharge current.

Cell Voltage Probe - Study 1 (bnd1)

1 In the **Model Builder** window, under **Component 1 (comp1)>Definitions** click **Cell Voltage Probe - Study 1 (bnd1)**.

2 In the **Settings** window for **Boundary Probe**, click to expand the **Table and Window Settings** section.

Cell Voltage Probe - Study 2

1 Right-click **Component 1 (comp1)>Definitions>Cell Voltage Probe - Study 1 (bnd1)** and choose **Duplicate**.

2 In the **Settings** window for **Boundary Probe**, type Cell Voltage Probe - Study 2 in the **Label** text field.

3 Locate the **Table and Window Settings** section. From the **Output table** list, choose **New table**.

4 From the **Plot window** list, choose **New window**.

ADD STUDY

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

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

3 Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces>Time Dependent with Initialization**.

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

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

STUDY 2

Step 2: Time Dependent

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

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

3 In the **Output times** text field, type range(0,30,90) 105.

4 Click to expand the **Results While Solving** section. From the **Probes** list, choose **Manual**.

5 In the **Probes** list, select **Cell Voltage Probe - Study 1 (bnd1)**.

6 Under **Probes**, click ⊟ **Delete**.

7 Locate the **Physics and Variables Selection** section. Select the **Modify model configuration for study step** check box.

8 In the tree, select **Component 1 (Comp1)>Lithium-Ion Battery (Liion)> Electrode Current Density - 1C Discharge**.

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

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

11 In the **Settings** window for **Study**, type Study 2 - 10 C Discharge in the **Label** text field.

12 Locate the **Study Settings** section. Clear the **Generate default plots** check box.

**13** In the **Home** toolbar, click ▭ **Compute**.

RESULTS

Electrolyte Potential (liion)

1 In the **Model Builder** window, under **Results** click **Electrolyte Potential (liion)**.

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

3 From the **Dataset** list, choose **Study 2 - 10 C Discharge/Solution 3 (sol3)**.

4 In the **Electrolyte Potential (liion)** toolbar, click 🔲 **Plot**.

Cell Voltage - Study 2

1 In the **Model Builder** window, under **Results** click **Probe Plot Group 10**.

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

Electrolyte Salt Concentration (liion)

1 In the **Model Builder** window, click **Electrolyte Salt Concentration (liion)**.

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

3 From the **Dataset** list, choose **Study 2 - 10 C Discharge/Solution 3 (sol3)**.

4 In the **Electrolyte Salt Concentration (liion)** toolbar, click 🔲 **Plot**.

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

Study 1 - 1 C Discharge/Solution 1 (4) (sol1)

1 In the **Model Builder** window, under **Results>Datasets** click **Study 1 - 1 C Discharge/ Solution 1 (4) (sol1)**.

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

3 From the **Solution** list, choose **Solution 3 (sol3)**.

Study 1 - 1 C Discharge/Solution 1 (5) (sol1)

1 In the **Model Builder** window, under **Results>Datasets** click **Study 1 - 1 C Discharge/ Solution 1 (5) (sol1)**.

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

3 From the **Solution** list, choose **Solution 3 (sol3)**.

Relative Li Concentration at Surface of Negative Electrode Particles

1 In the **Model Builder** window, under **Results** click
Relative Li Concentration at Surface of Negative Electrode Particles.

2 In the **Relative Li Concentration at Surface of Negative Electrode Particles** toolbar, click ⊙ **Plot**.

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

4 In the **Relative Li Concentration at Surface of Negative Electrode Particles** toolbar, click ⊙ **Plot**.

Relative Li Concentration at Surface of Positive Electrode Particles

1 In the **Model Builder** window, click
Relative Li Concentration at Surface of Positive Electrode Particles.

2 In the **Relative Li Concentration at Surface of Positive Electrode Particles** toolbar, click ⊙ **Plot**.

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

ROOT

Finally, perform a simulation of the relaxation phenomena occurring in the battery after discharge at zero net cell current. Use the end of the 1C discharge as initial values.

DEFINITIONS (COMP1)

Cell Voltage Probe - Study 3

1 In the **Model Builder** window, under **Component 1 (comp1)>Definitions** right-click
Cell Voltage Probe - Study 2 (bnd2) and choose **Duplicate**.

2 In the **Settings** window for **Boundary Probe**, type Cell Voltage Probe - Study 3 in the **Label** text field.

3 Locate the **Table and Window Settings** section. From the **Output table** list, choose
New table.

4 From the **Plot window** list, choose **New window**.

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

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

3 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies>Time Dependent**.

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

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

STUDY 3

Step 1: Time Dependent

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

2 In the **Output times** text field, type 0 10^range(-1,1,5).

3 Click to expand the **Results While Solving** section. From the **Probes** list, choose **Manual**.

4 In the **Probes** list, select **Cell Voltage Probe - Study 1 (bnd1)**.

5 Under **Probes**, click ≡ **Delete**.

6 Under **Probes**, click ≡ **Delete**.

7 Locate the **Physics and Variables Selection** section. Select the **Modify model configuration for study step** check box.

8 In the tree, select **Component 1 (Comp1)>Lithium-Ion Battery (Liion)>Electrode Current Density - 1C Discharge**.

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

10 In the tree, select **Component 1 (Comp1)>Lithium-Ion Battery (Liion)>Electrode Current Density - 10C Discharge**.

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

12 Click to expand the **Values of Dependent Variables** section. Find the **Initial values of variables solved for** subsection. From the **Settings** list, choose **User controlled**.

13 From the **Method** list, choose **Solution**.

14 From the **Study** list, choose **Study 1 - 1 C Discharge, Time Dependent**.

15 In the **Model Builder** window, click **Study 3**.

16 In the **Settings** window for **Study**, type Study 3 - Relaxation after 1C Discharge in the **Label** text field.

17 Locate the **Study Settings** section. Clear the **Generate default plots** check box.

18 In the **Home** toolbar, click ▬ **Compute**.

RESULTS

Study 2 - 10 C Discharge/Solution 3 (4) (sol3)

1 In the **Model Builder** window, under **Results>Datasets** click **Study 2 - 10 C Discharge/Solution 3 (4) (sol3)**.

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

3 From the **Solution** list, choose **Solution 5 (sol5)**.

Study 2 - 10 C Discharge/Solution 3 (5) (sol3)

1 In the **Model Builder** window, under **Results>Datasets** click **Study 2 - 10 C Discharge/Solution 3 (5) (sol3)**.

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

3 From the **Solution** list, choose **Solution 5 (sol5)**.

Electrolyte Salt Concentration (liion)

1 In the **Model Builder** window, under **Results** click **Electrolyte Salt Concentration (liion)**.

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

3 From the **Dataset** list, choose **Study 3 - Relaxation after 1C Discharge/Solution 5 (8) (sol5)**.

4 In the **Electrolyte Salt Concentration (liion)** toolbar, click 🔳 **Plot**.

5 Click 🔳 **Plot**.

Electrolyte Potential (liion)

1 In the **Model Builder** window, click **Electrolyte Potential (liion)**.

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

3 From the **Dataset** list, choose **Study 3 - Relaxation after 1C Discharge/Solution 5 (8) (sol5)**.

4 In the **Electrolyte Potential (liion)** toolbar, click 🔳 **Plot**.

Electrolyte Salt Concentration (liion)

1 In the **Model Builder** window, click **Electrolyte Salt Concentration (liion)**.

2 In the **Electrolyte Salt Concentration (liion)** toolbar, click 🔳 **Plot**.

Relative Li Concentration at Surface of Negative Electrode Particles

1 In the **Model Builder** window, click
Relative Li Concentration at Surface of Negative Electrode Particles.

2 In the **Relative Li Concentration at Surface of Negative Electrode Particles** toolbar, click
🔳 **Plot**.

3 Click ⬛ **Plot**.

Relative Li Concentration at Surface of Positive Electrode Particles

1 In the **Model Builder** window, click
   Relative Li Concentration at Surface of Positive Electrode Particles.

2 In the **Relative Li Concentration at Surface of Positive Electrode Particles** toolbar, click
   ⬛ **Plot**.

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