

Edge Effects in a Spirally Wound Lithium-Ion Battery

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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 lithiumion 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.

Time=1800 s Relative Li Concentration at Surface of Negative Electrode Particles

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.

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.

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

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

GLOBAL DEFINITIONS

Parameters 1

- I In the Model Builder window, under Global Definitions click Parameters I.
- 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 I (an I)

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

- I 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)

- I Right-click Analytic I (spiralX) 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 I

Now draw the spiral, consisting of eight different layers.

Parametric Curve 1 (pc1)

- I 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 틤 Build Selected.

Parametric Curve 2 (pc2)

- I Right-click Parametric Curve I (pcl) 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 틤 Build Selected.

Parametric Curve 3 (pc3)

- I 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 틤 Build Selected.

Parametric Curve 4 (pc4)

- I 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)

- I 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)

- I 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)

- I 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 틤 Build Selected.

Parametric Curve 8 (pc8)

- I 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 틤 Build Selected.

Parametric Curve 9 (pc9)

- I 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 틤 Build Selected.

Convert to Solid I (csoll)

- I 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 I (c1)

- I In the **Geometry** toolbar, click \bigcirc **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

- I In the **Definitions** toolbar, click **here 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

- I In the **Definitions** toolbar, click **here 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

- I In the **Definitions** toolbar, click here **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

- I In the **Definitions** toolbar, click http://www.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

- I In the **Definitions** toolbar, click **here 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

- I 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

- I 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

- I In the **Definitions** toolbar, click **here 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

- I 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

- I In the **Definitions** toolbar, click
- 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

- I 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)

- I In the Model Builder window, under Component I (compl)>Materials click Aluminum (matl).
- 2 In the Settings window for Material, locate the Geometric Entity Selection section.
- **3** From the Selection list, choose Positive current collector.

Copper (mat2)

- I 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.

- I Go to the Add Material window.
- 2 In the tree, select Battery>Electrolytes>LiPF6 in 1:2 EC:DMC and p(VdF-HFP) (Polymer, Liion 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)

- I In the Model Builder window, under Component I (compl)>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

- I In the Model Builder window, under Component I (compl) 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_1 text field, type epsl_neg.

Particle Intercalation 1

- I In the Model Builder window, click Particle Intercalation I.
- 2 In the Settings window for Particle Intercalation, locate the Material section.
- 3 From the Particle material list, choose Graphite, LixC6 MCMB (Negative, Liion 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 np_neg .
- 6 Click to expand the Particle Discretization section. In the $N_{\rm el}$ text field, type 3.

Porous Electrode Reaction I

- I In the Model Builder window, click Porous Electrode Reaction I.
- 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 iOref_neg.
- **5** In the α_a text field, type aA_neg.
- **6** In the α_c text field, type aC_neg.

Porous Electrode 2

- I 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_1 text field, type eps1_pos.

Particle Intercalation 1

- I In the Model Builder window, click Particle Intercalation I.
- 2 In the Settings window for Particle Intercalation, locate the Material section.
- 3 From the Particle material list, choose LMO, LiMn2O4 Spinel (Positive, Liion 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 $N_{\rm el}$ text field, type 5.

Porous Electrode Reaction I

- I In the Model Builder window, click Porous Electrode Reaction I.
- 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 $i_{0,ref}(T)$ text field, type iOref_pos.
- **5** In the α_a text field, type aA_pos.
- **6** In the α_c text field, type aC_pos.

Electrode I

- I 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

- I 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

- I 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 - IC Discharge

- I 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 $i_{n,s}$ 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.

I Right-click Electrode Current Density - IC 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 $i_{n,s}$ 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 I

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 I

- I In the Mesh toolbar, click \triangle Edge.
- **2** Select Boundaries 9 and 17 only.

Distribution I

- I Right-click Edge I 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

- I In the Mesh toolbar, click 🛕 Edge.
- **2** Select Boundaries 5 and 13 only.

Distribution I

- I 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

- I In the Mesh toolbar, click 🛕 Edge.
- **2** Select Boundaries 11 and 19 only.

Distribution I

- I 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

- I In the Mesh toolbar, click A Edge.
- **2** Select Boundaries 7 and 15 only.

Distribution I

- I 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

- I 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 I

- I 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 I

- I 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

- I In the Mesh toolbar, click Kree Triangular.
- 2 In the Model Builder window, right-click Mesh I and choose Build All.

DEFINITIONS (COMPI)

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

Cell Voltage Probe - Study I

- I 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 I (compl)>Lithium-Ion Battery>phis Electric potential V.

STUDY I

Step 2: Time Dependent

- I In the Model Builder window, under Study I 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 I (comp1)>Lithium-Ion Battery (liion)> Electrode Current Density - IOC Discharge.
- 6 Right-click and choose Disable.
- 7 In the Model Builder window, click Study I.
- 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)

- I 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

- I In the Model Builder window, expand the Electrolyte Salt Concentration (liion) node.
- 2 Right-click Surface I and choose Height Expression.
- **3** In the **Electrolyte Salt Concentration (liion)** toolbar, click **O** Plot.

Electrolyte Potential (liion)

I 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

- I In the Model Builder window, expand the Electrolyte Potential (liion) node.
- 2 Right-click Surface I and choose Height Expression.
- 3 In the Electrolyte Potential (liion) toolbar, click 🗿 Plot.

Cell Voltage - Study I

- I In the Model Builder window, under Results click Probe Plot Group 7.
- 2 In the Settings window for ID Plot Group, type Cell Voltage Study 1 in the Label text field.
- 3 In the Cell Voltage Study I toolbar, click 🗿 Plot.

Study I - I C Discharge/Solution I (4) (soll)

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

Selection

- I 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 I - I C Discharge/Solution I (5) (soll)

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

Selection

- I 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

- I 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 I - I C Discharge/ Solution I (4) (sol1).

Surface 1

- I 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 I (compl)>Lithiumlon Battery>Particle intercalation>liion.socloc_surface - Local electrode material state-ofcharge, particle surface.

Height Expression 1

- I Right-click Surface I and choose Height Expression.
- In the Relative Li Concentration at Surface of Negative Electrode Particles toolbar, click
 Plot.

Relative Li Concentration at Surface of Positive Electrode Particles

- I 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 I I C Discharge/ Solution I (5) (sol1).
- 4 Locate the Title section. From the Title type list, choose Label.

Surface 1

- I 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 I (compl)>Lithium-Ion Battery>Particle intercalation>liion.socloc_surface - Local electrode material state-ofcharge, particle surface.

Height Expression 1

- I Right-click Surface I and choose Height Expression.
- 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.

DEFINITIONS (COMPI)

Cell Voltage Probe - Study I (bnd I)

- In the Model Builder window, under Component I (compl)>Definitions click
 Cell Voltage Probe Study I (bndl).
- 2 In the Settings window for Boundary Probe, click to expand the Table and Window Settings section.

Cell Voltage Probe - Study 2

- I Right-click Component I (comp1)>Definitions>Cell Voltage Probe Study I (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

- I In the Home toolbar, click $\sim\sim$ 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 ~ 1 Add Study to close the Add Study window.

STUDY 2

Step 2: Time Dependent

- I 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 I (bndI).
- 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 I (comp1)>Lithium-Ion Battery (liion)> Electrode Current Density - IC Discharge.
- 9 Right-click and choose Disable.
- **IO** In the **Model Builder** window, click **Study 2**.
- II 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.
- **I3** In the **Home** toolbar, click **= Compute**.

RESULTS

Electrolyte Potential (liion)

- I 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 **O** Plot.

Cell Voltage - Study 2

- I In the Model Builder window, under Results click Probe Plot Group 10.
- 2 In the Settings window for ID Plot Group, type Cell Voltage Study 2 in the Label text field.

Electrolyte Salt Concentration (liion)

- I 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 **Click the Com Extents** button in the **Graphics** toolbar.

Study I - I C Discharge/Solution I (4) (soll)

- I In the Model Builder window, under Results>Datasets click Study I I C Discharge/ Solution I (4) (soll).
- 2 In the Settings window for Solution, locate the Solution section.
- **3** From the Solution list, choose Solution **3** (sol3).

Study I - I C Discharge/Solution I (5) (soll)

- I In the Model Builder window, under Results>Datasets click Study I I C Discharge/ Solution I (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

- In the Model Builder window, under Results click
 Relative Li Concentration at Surface of Negative Electrode Particles.
- In the Relative Li Concentration at Surface of Negative Electrode Particles toolbar, click
 Plot.
- **3** Click the \longleftrightarrow **Zoom Extents** button in the **Graphics** toolbar.
- In the Relative Li Concentration at Surface of Negative Electrode Particles toolbar, click
 Plot.

Relative Li Concentration at Surface of Positive Electrode Particles

I 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 **Figure 2000 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 (COMPI)

Cell Voltage Probe - Study 3

- In the Model Builder window, under Component I (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.

ADD STUDY

- I In the Home toolbar, click 2 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 2 Add Study to close the Add Study window.

STUDY 3

- Step 1: Time Dependent
- I 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 Locate the Results While Solving section. From the Probes list, choose Manual.
- 4 In the Probes list, select Cell Voltage Probe Study I (bndI).
- 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 I (comp1)>Lithium-Ion Battery (liion)> Electrode Current Density - IC Discharge.
- 9 Right-click and choose Disable.
- 10 In the tree, select Component I (compl)>Lithium-Ion Battery (liion)> Electrode Current Density - IOC Discharge.
- II 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.
- **I3** From the **Method** list, choose **Solution**.
- 14 From the Study list, choose Study I I C Discharge, Time Dependent.
- **I5** In the **Model Builder** window, click **Study 3**.
- I6 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)

- I 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)

- I 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)

- I 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 IC Discharge/Solution 5 (8) (sol5).
- **4** In the **Electrolyte Salt Concentration (liion)** toolbar, click **O** Plot.
- 5 Click 💽 Plot.

Electrolyte Potential (liion)

- I 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 IC Discharge/Solution 5 (8) (sol5).
- **4** In the **Electrolyte Potential (liion)** toolbar, click **O** Plot.

Electrolyte Salt Concentration (liion)

- I 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

I In the Model Builder window, click

Relative Li Concentration at Surface of Negative Electrode Particles.

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

I 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.

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