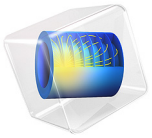


Heterogeneous Lithium-Ion Battery

Introduction

Most lithium-ion battery models make use of a homogenized domain formulation of the porous electrodes, which solve simultaneously for the electrode phase and electrolyte phase potentials in the same domain, defining the electrode reactions by the use of source terms. In these models, the diffusion of lithium into the solid electrode particles is modeled by the use of an extra dimension, representing an average particle for a certain position in the electrode. This modeling approach has great advantages in terms of a relatively small computational load, allowing most models to be formulated in one dimension only, representing the electrode depth (plus the extra dimension for defining the particle diffusion dimension).

However, certain phenomena cannot be captured using the above approach. For instance, the above particle diffusion model inherently assumes either Cartesian, cylindrical, or spherical symmetry, thus not allowing modeling the impact of irregular particle shapes, nor the impact of micro- and macropore distributions.

The instead of homogenizing the porous electrode, you can instead include the structural details of the porous electrodes in the model geometry. Such models are referred to as heterogeneous models.

This tutorial describes the behavior of a lithium-ion battery unit cell modeled using a three-dimensional geometry, where a number of ellipses are used to define the electrode particles in the two electrodes. The model can be used as a starting point for modeling more realistic electrode geometries, for instance based on tomography data.

This tutorial also demonstrates how to couple the lithium concentration distribution in the particles to a corresponding volumetric expansion in the Solid Mechanics interface and the resulting von Mises stresses.

Model Definition

The model geometry is shown in Figure 1. The geometry consists of a rectangular block, forming a representative unit cell of the model geometry. The two electrodes are defined using a number of ellipses.

The battery chemistry is modeled using a **Lithium-Ion Battery** interface using the **Electrolyte** node to define the concentrated battery electrolyte charge and ion transport. Two **Electrode** nodes are used to define the ohmic drop due to the current conduction in each electrode phase. On the interior boundaries between the electrode and electrolyte phases, **Internal Electrode Surface** nodes are used to define the charge transfer reactions. Transport

of solid lithium in the electrode phases is modeled using a separate **Transport of Diluted Species** interface, which defines the molecular flux of lithium according to Fick's law. **Electrode Surface Coupling** nodes define the molecular flux on the external boundaries to the electrode particles, stemming from the electrochemical reactions.

The concentration of solid lithium is coupled to the **Lithium Insertion Reaction** electrode kinetics, defined in the **Electrode Reaction** subnodes to the **Internal Electrode Surface** nodes.

As the lithium concentration increases in the negative graphite electrode material, the material expands. This is modeled using a **Solid Mechanics** interface, where expansion is defined as an initial strain in the **Initial Stress and Strain** node (subnode to the **Linear-Elastic Material** node). The expansion is defined as a function of the local solid lithium concentration using an interpolation function, based on experimental data (Ref. 1).

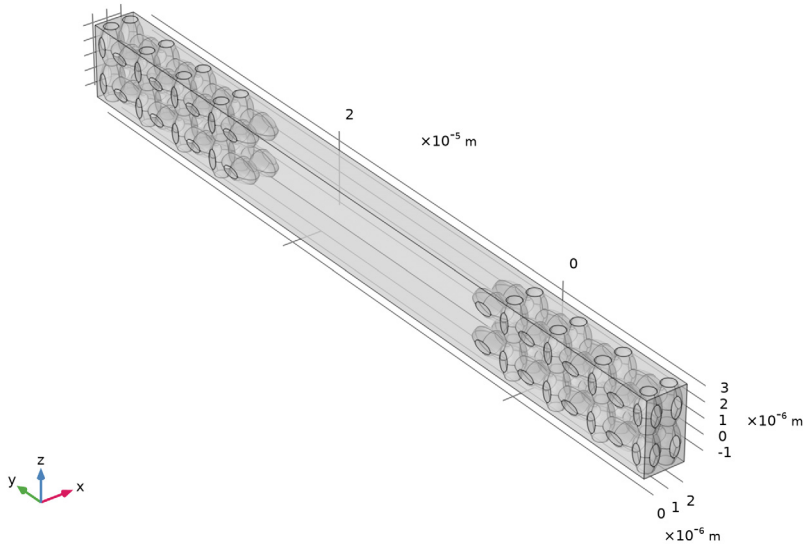


Figure 1: Model geometry. The negative graphite electrode located toward the upper left and the positive LCO electrode is located toward the lower right in the figure.

The model is solved using two different studies. The first, time-dependent study, simulates a high-rate discharge during 20 s, solving for the Lithium-Ion Battery and Transport of Diluted Species interfaces only. The second, stationary study, solves for the Solid

Mechanics interface only, using the results of Study 1 for the concentration distribution in the battery at 0 and 20 s as input.

Results and Discussion

Figure 2 shows the solid lithium concentration in the particles after 90 s of discharge. For the negative electrode, the solid lithium concentration is generally lower toward the electrolyte and higher toward the current collector — reflecting what parts of the electrode surface are more accessible for charge transfer. A similar trend is seen for the positive electrode.

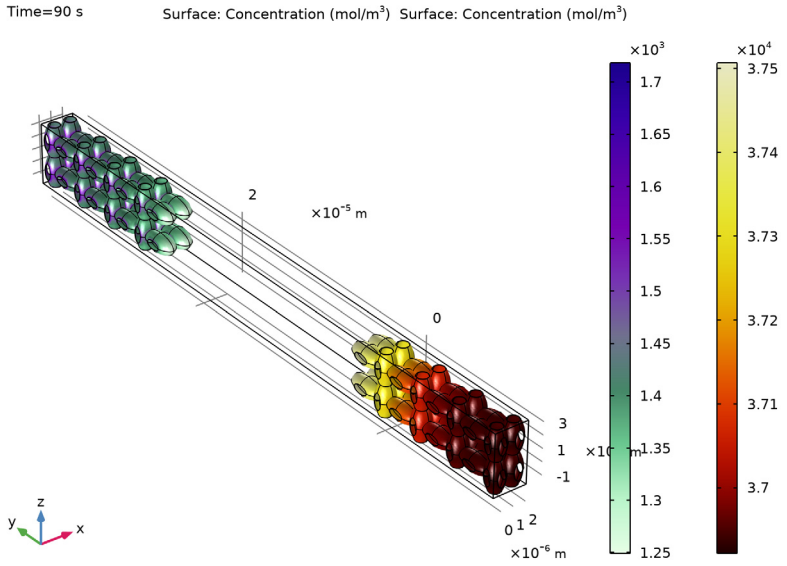


Figure 2: Surface concentration of solid lithium at the surface at the electrode particles at t=90 s.

Figure 3 shows a slice plot of the solid lithium concentration at 90 s, demonstrating a significant concentration gradient from the center of the particles toward the surface.

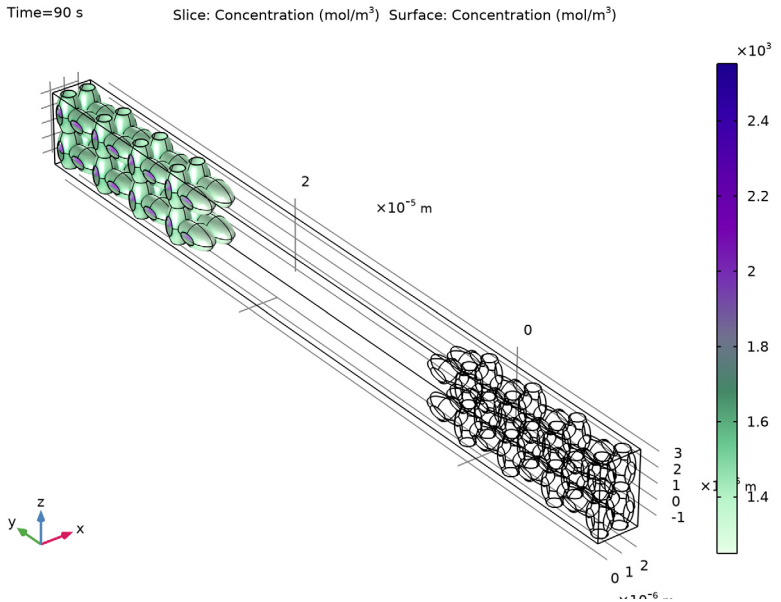


Figure 3: Slice plot of the solid lithium concentration in the negative electrode at t = 90 s.

Figure 4 shows the current distribution in the electrolyte at the same time. The maximum values of the reaction current density at 90 s is located in the negative electrode at the parts of the surface with the highest solid lithium concentration values (see Figure 2).

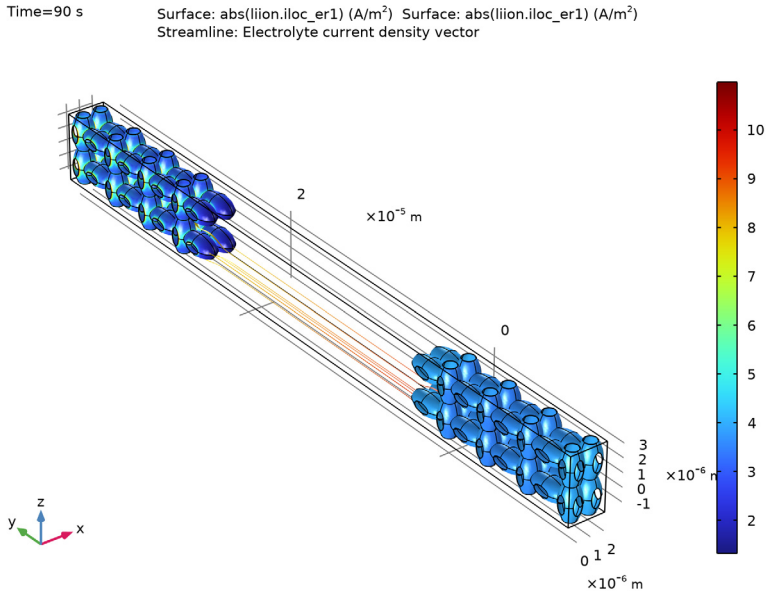


Figure 4: Electrolyte current density magnitude at t=90 s.

Finally, Figure 5 shows the resulting von Mises stresses, based on the graphite lithium concentration at t = 90 s, in combination with the experimental expansion function.

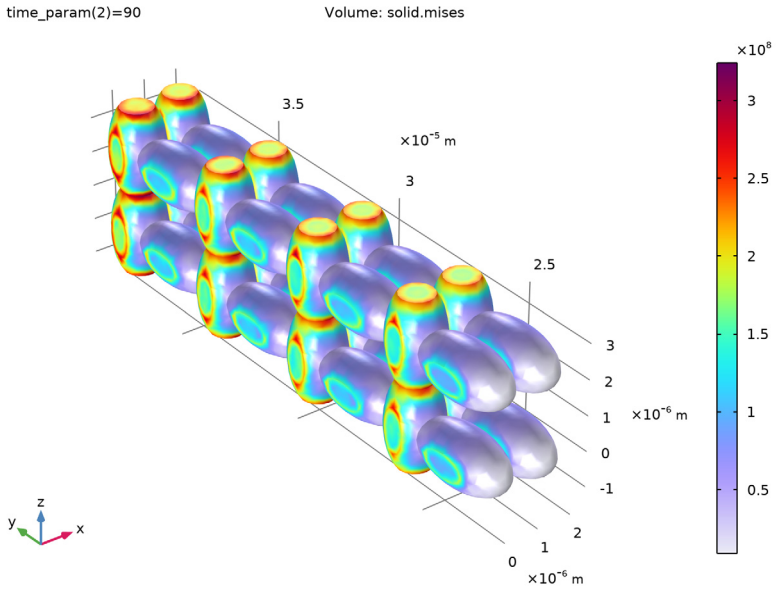


Figure 5: The von Mises stress at the surface of the negative graphite particles at t = 90 s.

Reference

1. J.B. Siegel, A.G. Stefanopoulou, P. Hagans, Y. Ding, and D. Gorsich, *J. Electrochemical Soc.*, vol. 160, p. A1031, 2013.

Application Library path: `Battery_Design_Module/Batteries,_Heterogeneous/heterogeneous_li_battery`

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 **3D**.

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 In the **Concentrations** table, enter the following settings:

cs

7 Click **Study**.

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

9 Click **Done**.

GEOMETRY 1

Insert a prepared geometry sequence from a file. You can follow the steps required to build the geometry in the section Appendix — Geometry Modeling Instructions.

1 In the **Geometry** toolbar, click **Insert Sequence** and choose **Insert Sequence**.

2 Browse to the model's Application Libraries folder and double-click the file `heterogeneous_li_battery_geom_sequence.mph`.

3 In the **Geometry** toolbar, click **Build All**.

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

GEOMETRY 1

In the **Model Builder** window, collapse the **Component 1 (comp1)>Geometry 1** node.

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 In the table, enter the following settings:

Name	Expression	Value	Description
csmax_neg	31507[mol/m^3]	31507 mol/m³	Maximum lithium concentration in graphite
i0ref_neg	0.96[A/m^2]	0.96 A/m²	Reference exchange current density negative
i0ref_pos	1.72[A/m^2]	1.72 A/m²	Reference exchange current density positive
exp_max	10[%]	0.1	
time_param	1	1	Time parameter for parametric sweep

DEFINITIONS

Variables 1

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

2 Right-click **Definitions** and choose **Variables**.

3 In the **Settings** window for **Variables**, locate the **Variables** section.

4 Click **Load from File**.

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

ADD MATERIAL

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

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

Add the electrolyte first, then graphite, and finally LCO. The order is important since it will determine the tags (`mat1`, `mat2`, and `mat3`) the added material nodes get in the model tree. These tags will be used later in certain variable declarations.

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

4 Click **Component 1 (comp1)** in the window toolbar.

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

6 Click **Component 1 (comp1)** in the window toolbar.

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

8 Click **Component 1 (comp1)** in the window toolbar.

9 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) (mat1)

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

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

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**.

LCO, LiCoO2 (Positive, Li-ion Battery) (mat3)

1 In the **Model Builder** window, click **LCO, LiCoO2 (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**.

LITHIUM-ION BATTERY (LIION)

Electrolyte 1

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

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

3 From the **Electrolyte material** list, choose **LiPF6 in 1:2 EC:DMC and p(VdF-HFP) (Polymer, Li-ion Battery) (mat1)**.

Initial Values - Negative and Electrolyte

1 In the **Model Builder** window, click **Initial Values 1**.

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

3 In the *phil* text field, type `phil_init`.

4 In the **Label** text field, type `Initial Values - Negative and Electrolyte`.

Initial Values - Positive

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 **Positive electrode**.

4 In the **Label** text field, type `Initial Values - Positive`.

5 Locate the **Initial Values** section. In the *phil* text field, type `phil_init`.

6 In the *phis* text field, type `E_cell_init`.

Electrode - Negative

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

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

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

Electrode - Positive

1 Right-click **Electrode - Negative** and choose **Duplicate**.

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

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

4 In the **Label** text field, type `Electrode - Positive`.

Internal Electrode Surface 1

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

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

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

Electrode Reaction 1

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

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

3 From the *c* list, choose **Concentration (tds)**.

4 Locate the **Electrode Kinetics** section. From the **Kinetics expression type** list, choose **Lithium insertion**.

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

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

Internal Electrode Surface 1

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

Double Layer Capacitance 1

In the **Physics** toolbar, click **Attributes** and choose **Double Layer Capacitance**.

Internal Electrode Surface - Negative

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

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

Internal Electrode Surface - Positive

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

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

Electrode Reaction 1

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

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

3 From the c list, choose **Concentration (tds)**.

4 Locate the **Electrode Kinetics** section. From the **Kinetics expression type** list, choose **Lithium insertion**.

5 Locate the **Material** section. From the **Material** list, choose **LCO, LiCoO2 (Positive, Li-ion Battery) (mat3)**.

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

Internal Electrode Surface - Positive

In the **Model Builder** window, click **Internal Electrode Surface - Positive**.

Double Layer Capacitance 1

In the **Physics** toolbar, click **Attributes** and choose **Double Layer Capacitance**.

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 current collector**.

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 **Positive current collector**.

4 Locate the **Electrode Current** section. In the $I_{s,total}$ text field, type `-1e-9[A]`.

5 In the $\phi_{s,bnd,init}$ text field, type `E_cell_init`.

DEFINITIONS

phis

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

2 In the **Settings** window for **Boundary Probe**, type `phis` in the **Label** text field.

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

4 Click **Clear Selection**.

5 Click **Paste Selection**.

6 In the **Paste Selection** dialog box, type `210` in the **Selection** text field.

7 Click **OK**.

8 In the **Settings** window for **Boundary Probe**, locate the **Expression** section.

9 In the **Expression** text field, type `phis`.

TRANSPORT OF DILUTED SPECIES (TDS)

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

2 Select Domains 2 and 3 only.

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

4 Clear the **Convection** check box.

5 Click to expand the **Discretization** section. From the **Concentration** list, choose **Quadratic**.

Transport Properties - Negative

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

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

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

4 From the D_{cs} list, choose **Basic (def)**.

Initial Values - Negative

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

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

3 Locate the **Initial Values** section. In the *cs* text field, type `csinit_neg`.

Transport Properties - Positive

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

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

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

4 Locate the **Diffusion** section. From the **Material** list, choose **LCO, LiCoO2 (Positive, Li-ion Battery) (mat3)**.

5 From the D_{cs} list, choose **Basic (def)**.

Initial Values - Positive

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

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

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

4 Locate the **Initial Values** section. In the *cs* text field, type `csinit_pos`.

Electrode Surface Coupling 1

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

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

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

Reaction Coefficients 1

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

2 In the **Settings** window for **Reaction Coefficients**, locate the **Model Inputs** 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_{cs} text field, type `1`.

Electrode Surface Coupling 2

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

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

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

Reaction Coefficients 1

1 In the **Model Builder** window, expand the **Electrode Surface Coupling 2** node, then click **Reaction Coefficients 1**.

2 In the **Settings** window for **Reaction Coefficients**, locate the **Model Inputs** section.

3 From the i_{loc} list, choose **Local current density, Electrode Reaction 1 (liion/bei2/er1)**.

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

MESH 1

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

2 In the **Settings** window for **Mesh**, locate the **Physics-Controlled Mesh** section.

3 From the **Element size** list, choose **Coarse**.

Free Tetrahedral 1

1 In the **Mesh** toolbar, click **Free Tetrahedral**.

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

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

4 Click **Paste Selection**.

5 In the **Paste Selection** dialog box, type `2 3` in the **Selection** text field.

6 Click **OK**.

Size 1

1 Right-click **Free Tetrahedral 1** and choose **Size**.

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

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

4 Locate the **Element Size** section. From the **Predefined** list, choose **Fine**.

Size 2

1 In the **Model Builder** window, right-click **Free Tetrahedral 1** and choose **Size**.

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

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

4 Locate the **Element Size** section. From the **Predefined** list, choose **Fine**.

Free Tetrahedral 2

In the **Mesh** toolbar, click **Free Tetrahedral**.

Size 1

1 Right-click **Free Tetrahedral 2** and choose **Size**.

2 In the **Settings** window for **Size**, locate the **Element Size** section.

3 From the **Predefined** list, choose **Finer**.

4 Click **Build All**.

STUDY 1 - DISCHARGE

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

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

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

Solution 1 (sol1)

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

Step 1: Current Distribution Initialization

1 In the **Model Builder** window, under **Study 1 - Discharge** 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. In the table, clear the **Solve for** check box for **Transport of Diluted Species (tds)**.

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 `range(0,5,90)`.

4 From the **Tolerance** list, choose **User controlled**.

5 In the **Relative tolerance** text field, type `1e-4`.

Solution 1 (sol1)

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

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

3 In the **Settings** window for **Time-Dependent Solver**, click to expand the **Time Stepping** section.

4 Find the **Algebraic variable settings** subsection. From the **Consistent initialization** list, choose **Off**.

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

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

RESULTS

Cell Voltage

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

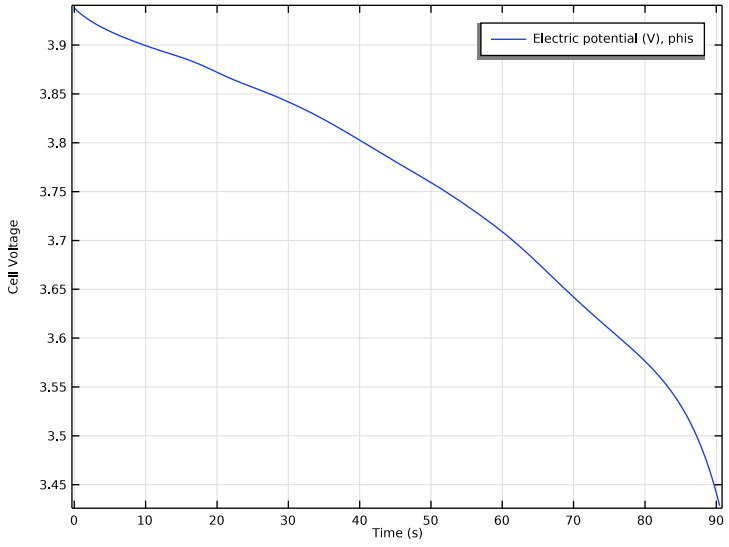
2 Locate the **Plot Settings** section.

3 Select the **y-axis label** check box. In the associated text field, type `Cell Voltage`.

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

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

The plot should look as shown below:



Electrolyte Salt Concentration (liion)

1 In the **Home** toolbar, click **Add Plot Group** and choose **3D Plot Group**.

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

Surface 1

1 Right-click **Electrolyte Salt Concentration (liion)** and choose **Surface**.

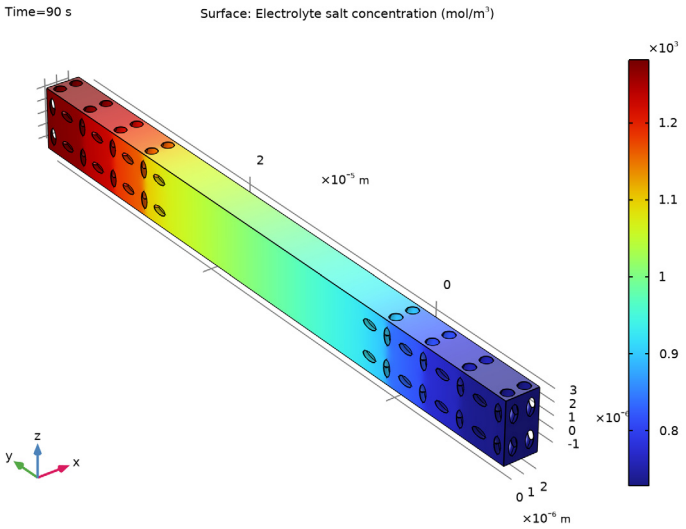
2 In the **Settings** window for **Surface**, locate the **Expression** section.

3 In the **Expression** text field, type `cl`.

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

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

The plot should look as shown below:



Electrolyte Potential (liion)

1 In the **Home** toolbar, click **Add Plot Group** and choose **3D Plot Group**.

2 In the **Settings** window for **3D Plot Group**, type `Electrolyte Potential (liion)` in the **Label** text field.

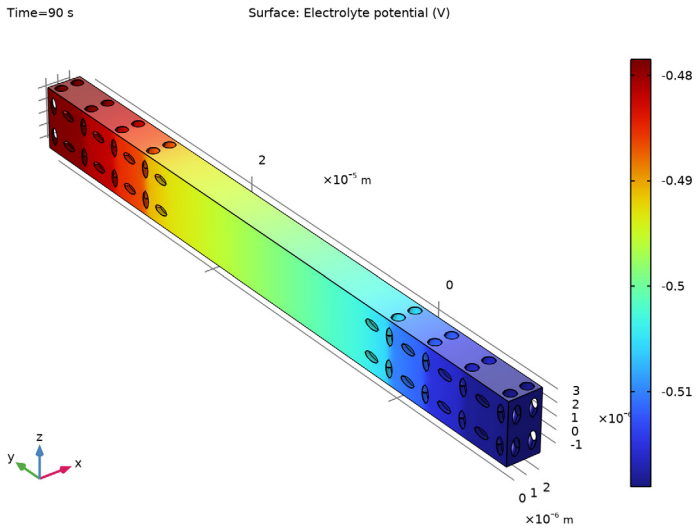
Surface 1

1 Right-click **Electrolyte Potential (liion)** and choose **Surface**.

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

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

The plot should look as shown below:



Lithium Concentration Surface (tds)

The following steps reproduce the figures in the Results and Discussion section.

1 In the **Home** toolbar, click **Add Plot Group** and choose **3D Plot Group**.

2 In the **Settings** window for **3D Plot Group**, type `Lithium Concentration Surface (tds)` in the **Label** text field.

Negative Electrode

1 Right-click **Lithium Concentration Surface (tds)** and choose **Surface**.

2 In the **Settings** window for **Surface**, locate the **Coloring and Style** section.

3 Click **Change Color Table**.

4 In the **Color Table** dialog box, select **Aurora>AuroraBorealis** in the tree.

5 Click **OK**.

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

7 Locate the **Expression** section. In the **Expression** text field, type `cs`.

Selection 1

1 Right-click **Negative Electrode** and choose **Selection**.

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

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

4 In the **Lithium Concentration Surface (tds)** toolbar, click **Plot**.

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

Positive Electrode

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

2 In the **Settings** window for **Surface**, locate the **Coloring and Style** section.

3 Click **Change Color Table**.

4 In the **Color Table** dialog box, select **Thermal>ThermalDark** in the tree.

5 Click **OK**.

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

Selection 1

1 In the **Model Builder** window, expand the **Positive Electrode** node, then click **Selection 1**.

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

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

4 In the **Lithium Concentration Surface (tds)** toolbar, click **Plot**.

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

Current Distribution

1 In the **Home** toolbar, click **Add Plot Group** and choose **3D Plot Group**.

2 In the **Settings** window for **3D Plot Group**, type `Current Distribution` in the **Label** text field.

Negative Electrode

1 Right-click **Current Distribution** and choose **Surface**.

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

3 In the **Expression** text field, type `abs(liion.iloc_er1)`.

4 In the **Label** text field, type `Negative Electrode`.

Selection 1

1 Right-click **Negative Electrode** and choose **Selection**.

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

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

4 In the **Current Distribution** toolbar, click **Plot**.

Positive Electrode

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

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

3 Click to expand the **Inherit Style** section. From the **Plot** list, choose **Negative Electrode**.

Selection 1

1 In the **Model Builder** window, expand the **Positive Electrode** node, then click **Selection 1**.

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

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

Streamline 1

1 In the **Model Builder** window, right-click **Current Distribution** and choose **Streamline**.

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

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

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

5 In the **Width expression** text field, type `liion.IlMag`.

6 Select the **Width scale factor** check box. In the associated text field, type `4e-10`.

7 Click to expand the **Quality** section. From the **Recover** list, choose **Within domains**.

Color Expression 1

1 Right-click **Streamline 1** and choose **Color Expression**.

2 In the **Settings** window for **Color Expression**, locate the **Coloring and Style** section.

3 Click  **Change Color Table**.

4 In the **Color Table** dialog box, select **Thermal>ThermalDark** in the tree.

5 Click **OK**.

6 In the **Settings** window for **Color Expression**, locate the **Coloring and Style** section.

7 Clear the **Color legend** check box.

8 In the **Current Distribution** toolbar, click  **Plot**.

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

Lithium Concentration in Negative Electrode

1 In the **Home** toolbar, click  **Add Plot Group** and choose **3D Plot Group**.

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

Slice 1

1 Right-click **Lithium Concentration in Negative Electrode** and choose **Slice**.

2 In the **Settings** window for **Slice**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)> Transport of Diluted Species>Species cs>cs - Concentration - mol/m³**.

3 Locate the **Plane Data** section. From the **Plane** list, choose **XY-planes**.

4 In the **Planes** text field, type 2.

5 Locate the **Coloring and Style** section. Click **Change Color Table**.

6 In the **Color Table** dialog box, select **Aurora>AuroraBorealis** in the tree.

7 Click **OK**.

Selection 1

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

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

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

Surface 1

1 In the **Model Builder** window, right-click **Lithium Concentration in Negative Electrode** 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)> Transport of Diluted Species>Species cs>cs - Concentration - mol/m³**.

3 Locate the **Inherit Style** section. From the **Plot** list, choose **Slice 1**.

Selection 1

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

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

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

4 In the **Lithium Concentration in Negative Electrode** toolbar, click **Plot**.

Setting up and solving for the heterogeneous battery is now complete. Next, extend the model to analyze the stresses and strains using the **Structural Mechanics** interface.

ADD PHYSICS

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

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

3 In the tree, select **Structural Mechanics>Solid Mechanics (solid)**.

4 Click **Add to Component 1** in the window toolbar.

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

SOLID MECHANICS (SOLID)

1 In the **Settings** window for **Solid Mechanics**, click to expand the **Dependent Variables** section.

2 Locate the **Domain Selection** section. From the **Selection** list, choose **Negative electrode**.

Linear Elastic Material 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Solid Mechanics (solid)** click **Linear Elastic Material 1**.

2 In the **Settings** window for **Linear Elastic Material**, locate the **Model Input** section.

3 From the *c* list, choose **Concentration (tds)**.

Intercalation Strain 1

1 In the **Physics** toolbar, click **Attributes** and choose **Intercalation Strain**.

The volumetric strain is taken **From material** by default. Couple the strain to the concentration solved for by the **Transport of Diluted Species** interface as follows:

2 In the **Settings** window for **Intercalation Strain**, locate the **Model Input** section.

3 From the *c* list, choose **Concentration (tds)**.

Roller 1

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

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

3 From the **Selection** list, choose **Roller condition boundaries**.

Prescribed Displacement 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Prescribed Displacement**.

2 In the **Settings** window for **Prescribed Displacement**, locate the **Boundary Selection** section.

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

4 Locate the **Prescribed Displacement** section. Select the **Prescribed in x direction** check box.

5 Select the **Prescribed in y direction** check box.

6 Select the **Prescribed in z direction** check box.

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 **General Studies>Stationary**.

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

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

STUDY 2 - EXPANSION AND STRESS

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

2 In the **Settings** window for **Study**, type `Study 2 - Expansion and Stress` in the **Label** text field.

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 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
time_param (Time parameter for parametric sweep)	0 90	

5 Locate the **Output While Solving** section. From the **Probes** list, choose **None**.

Step 1: Stationary

1 In the **Model Builder** window, click **Step 1: Stationary**.

2 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.

3 In the table, clear the **Solve for** check boxes for **Lithium-Ion Battery (liion)** and **Transport of Diluted Species (tds)**.

4 Click to expand the **Values of Dependent Variables** section. Find the **Values of variables not solved for** subsection. From the **Settings** list, choose **User controlled**.

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

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

7 From the **Solution** list, choose **Solution 1 (sol1)**.

8 From the **Time (s)** list, choose **Interpolated**.

9 In the **Time** text field, type `time_param`.

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

RESULTS

Stress (solid)

The **Stress (solid)** plot group shows the result for the von Mises stress on the particles experienced during the intercalation reaction at t = 90 s.

Appendix — Geometry 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 **3D**.

2 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 **Clear Table**.

4 Click **Load from File**.

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

6 Click the **Transparency** button in the **Graphics** toolbar.

GEOMETRY 1

Ellipsoid 1 (elp1)

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

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

3 In the **a-semiaxis** text field, type `Rp*1.5/3*pr_pos+Rp*(1-pr_pos)`.

4 In the **b-semiaxis** text field, type `Rp*1.5/3`.

5 In the **c-semiaxis** text field, type `Rp*pr_pos+Rp*1.5/3*(1-pr_pos)`.

6 Locate the **Position** section. In the **y** text field, type `6.5e-7*pr_pos`.

7 Locate the **Axis** section. From the **Axis type** list, choose **y-axis**.

8 Right-click **Ellipsoid 1 (elp1)** and choose **Copy**.

Copy 1 (copy1)

1 In the **Geometry** toolbar, click **Transforms** and choose **Copy**.

2 Select the object **elp1** only.

3 In the **Settings** window for **Copy**, locate the **Displacement** section.

4 In the **x** text field, type `Rp*0.9`.

Ellipsoid 2 (elp2)

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

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

3 In the **a-semiaxis** text field, type `Rp*1.5/3`.

4 In the **b-semiaxis** text field, type `Rp*1.5/3*pr_pos+Rp*(1-pr_pos)`.

5 In the **c-semiaxis** text field, type `Rp*pr_pos+Rp*1.5/3*(1-pr_pos)`.

6 Locate the **Position** section. In the **y** text field, type `Rp*1.2+6.5e-7*pr_pos`.

Copy 2 (copy2)

1 In the **Geometry** toolbar, click **Transforms** and choose **Copy**.

2 Select the object **elp2** only.

3 In the **Settings** window for **Copy**, locate the **Displacement** section.

4 In the **x** text field, type `Rp*0.9`.

Copy 3 (copy3)

1 In the **Geometry** toolbar, click **Transforms** and choose **Copy**.

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

3 In the **Settings** window for **Copy**, locate the **Displacement** section.

4 In the **z** text field, type `Rp*1.6`.

5 Click **Build Selected**.

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

Copy 4 (copy4)

1 In the **Geometry** toolbar, click **Transforms** and choose **Copy**.

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

3 In the **Settings** window for **Copy**, locate the **Displacement** section.

4 In the **y** text field, type `-Rp*1.23*2`.

Copy 5 (copy5)

1 In the **Geometry** toolbar, click **Transforms** and choose **Copy**.

2 Select the objects **copy1**, **copy2**, **copy3(1)**, **copy3(2)**, **copy3(3)**, **copy3(4)**, **copy4(2)**, **copy4(5)**, **copy4(6)**, **copy4(7)**, **copy4(8)**, **elp1**, and **elp2** only.

3 Click the **Zoom to Selection** button in the **Graphics** toolbar.

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

5 In the **Settings** window for **Copy**, locate the **Displacement** section.

6 In the **y** text field, type `-Rp*1.23*4`.

7 Click **Build Selected**.

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

Ellipsoid 3 (elp3)

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

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

3 In the **a-semiaxis** text field, type `Rp*1.5/3*pr_neg+Rp*(1-pr_neg)`.

4 In the **b-semiaxis** text field, type `Rp*1.5/3`.

5 In the **c-semiaxis** text field, type `Rp*pr_neg+Rp*1.5/3*(1-pr_neg)`.

6 Locate the **Position** section. In the **y** text field, type `L_sep-5e-7*(1-pr_neg)`.

7 Locate the **Axis** section. From the **Axis type** list, choose **y-axis**.

8 Click **Build Selected**.

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

Copy 6 (copy6)

1 In the **Geometry** toolbar, click **Transforms** and choose **Copy**.

2 Select the object **elp3** only.

3 In the **Settings** window for **Copy**, locate the **Displacement** section.

4 In the **x** text field, type `Rp*0.9`.

5 Click **Build Selected**.

Ellipsoid 4 (elp4)

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

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

3 In the **a-semiaxis** text field, type `Rp*1.5/3`.

4 In the **b-semiaxis** text field, type `Rp*1.5/3*pr_neg+Rp*(1-pr_neg)`.

5 In the **c-semiaxis** text field, type `Rp*pr_neg+Rp*1.5/3*(1-pr_neg)`.

6 Locate the **Position** section. In the **y** text field, type `Rp*1.2+L_sep-5e-7*(1-pr_neg)`.

7 Click **Build Selected**.

Copy 7 (copy7)

1 In the **Geometry** toolbar, click **Transforms** and choose **Copy**.

2 Select the object **elp4** only.

3 In the **Settings** window for **Copy**, locate the **Displacement** section.

4 In the **x** text field, type `Rp*0.9`.

5 Click **Build Selected**.

Copy 8 (copy8)

1 In the **Geometry** toolbar, click **Transforms** and choose **Copy**.

2 Select the objects **copy6**, **copy7**, **elp3**, and **elp4** only.

3 In the **Settings** window for **Copy**, locate the **Displacement** section.

4 In the **z** text field, type `Rp*1.6`.

Copy 9 (copy9)

1 In the **Geometry** toolbar, click **Transforms** and choose **Copy**.

2 Select the objects **copy6**, **copy7**, **copy8(1)**, **copy8(2)**, **copy8(3)**, **copy8(4)**, **elp3**, and **elp4** only.

3 In the **Settings** window for **Copy**, locate the **Displacement** section.

4 In the **y** text field, type `Rp*1.23*2`.

5 Click **Build Selected**.

Copy 10 (copy10)

1 In the **Geometry** toolbar, click **Transforms** and choose **Copy**.

2 Select the objects **copy6**, **copy7**, **copy8(1)**, **copy8(2)**, **copy8(3)**, **copy8(4)**, **copy9(1)**, **copy9(2)**, **copy9(3)**, **copy9(4)**, **copy9(5)**, **copy9(6)**, **copy9(7)**, **copy9(8)**, **elp3**, and **elp4** only.

3 In the **Settings** window for **Copy**, locate the **Displacement** section.

4 In the **y** text field, type `Rp*1.23*4`.

5 Click **Build Selected**.

Block 1 (blk1)

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

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

3 In the **Width** text field, type `Rp*1.8`.

4 In the **Depth** text field, type `Rp*2.0889+L_sep+Rp*14.76`.

5 In the **Height** text field, type `Rp*3.2`.

6 Locate the **Position** section. In the **x** text field, type `-Rp*0.45`.

7 In the **y** text field, type `-Rp*4/9-Rp*7.38`.

8 In the **z** text field, type `-Rp*0.8`.

9 Click **Build Selected**.

Union 1 (uni1)

1 In the **Geometry** toolbar, click **Booleans and Partitions** and choose **Union**.

2 Select the object **blk1** only.

3 In the **Settings** window for **Union**, locate the **Union** section.

4 From the **Repair tolerance** list, choose **Relative**.

5 Click **Build Selected**.

Difference 1 (dif1)

1 In the **Geometry** toolbar, click **Booleans and Partitions** and choose **Difference**.

2 Select the object **uni1** only.

3 In the **Settings** window for **Difference**, locate the **Difference** section.

4 Click **Paste Selection**.

5 In the **Paste Selection** dialog box, type `copy1 copy10(1) copy10(2) copy10(3) copy10(4) copy10(5) copy10(6) copy10(7) copy10(8) copy10(9) copy10(10) copy10(11) copy10(12) copy10(13) copy10(14) copy10(15) copy10(16) copy2 copy3(1) copy3(2) copy3(3) copy3(4) copy4(1) copy4(2) copy4(3) copy4(4) copy4(5) copy4(6) copy4(7) copy4(8) copy5(1) copy5(2) copy5(3) copy5(4) copy5(5) copy5(6) copy5(7) copy5(8) copy5(9) copy5(10) copy5(11) copy5(12) copy5(13) copy5(14) copy5(15) copy5(16) copy6 copy7 copy8(1) copy8(2) copy8(3) copy8(4) copy9(1) copy9(2) copy9(3) copy9(4) copy9(5) copy9(6) copy9(7) copy9(8) elp1 elp2 elp3 elp4` in the **Selection** text field.

6 Click **OK**.

7 Select the objects **copy1**, **copy10(1)**, **copy10(10)**, **copy10(11)**, **copy10(12)**, **copy10(13)**, **copy10(14)**, **copy10(15)**, **copy10(16)**, **copy10(2)**, **copy10(3)**, **copy10(4)**, **copy10(5)**, **copy10(6)**, **copy10(7)**, **copy10(8)**, **copy10(9)**, **copy2**, **copy3(1)**, **copy3(2)**, **copy3(3)**, **copy3(4)**, **copy4(1)**, **copy4(2)**, **copy4(3)**, **copy4(4)**, **copy4(5)**, **copy4(6)**, **copy4(7)**, **copy4(8)**, **copy5(1)**, **copy5(10)**, **copy5(11)**, **copy5(12)**, **copy5(13)**, **copy5(14)**, **copy5(15)**, **copy5(16)**, **copy5(2)**, **copy5(3)**, **copy5(4)**, **copy5(5)**, **copy5(6)**, **copy5(7)**, **copy5(8)**, **copy5(9)**, **copy6**, **copy7**, **copy8(1)**, **copy8(2)**, **copy8(3)**, **copy8(4)**, **copy9(1)**, **copy9(2)**, **copy9(3)**, **copy9(4)**, **copy9(5)**, **copy9(6)**, **copy9(7)**, **copy9(8)**, **elp1**, **elp2**, **elp3**, and **elp4** only.

8 In the **Settings** window for **Difference**, locate the **Difference** section.

9 From the **Repair tolerance** list, choose **Relative**.

10 Click **Build Selected**.

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

Block 2 (blk2)

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

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

3 In the **Width** text field, type `Rp*1.8`.

4 In the **Depth** text field, type `Rp*2.0889+L_sep+Rp*14.76`.

5 In the **Height** text field, type `Rp*3.2`.

6 Locate the **Position** section. In the **x** text field, type `-Rp*0.45`.

7 In the **y** text field, type `-Rp*4/9-Rp*7.38`.

8 In the **z** text field, type `-Rp*0.8`.

9 Click **Build Selected**.

Form Union (fin)

1 In the **Model Builder** window, click **Form Union (fin)**.

2 In the **Settings** window for **Form Union/Assembly**, locate the **Form Union/Assembly** section.

3 From the **Repair tolerance** list, choose **Relative**.

4 Click **Build Selected**.

Electrolyte

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

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

3 On the object **fin**, select Domain 1 only.

Negative electrode

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

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

3 On the object **fin**, select Domain 3 only.

4 Click **Build Selected**.

Positive electrode

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

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

3 On the object **fin**, select Domain 2 only.

Negative electrode surface

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

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

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

4 On the object **fin**, select Boundaries 86, 87, 89–94, 96, 97, 99–104, 106, 107, 109–114, 116, 117, 119–124, 126, 127, 129–134, 136, 137, 139–144, 146, 147, 149–154, 156, 157, 159–164, 250–313, 378–441, and 526–589 only.

5 Click **Build Selected**.

Positive electrode surface

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

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

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

4 On the object **fin**, select Boundaries 6, 7, 9–14, 16, 17, 19–24, 26, 27, 29–34, 36, 37, 39–44, 46, 47, 49–54, 56, 57, 59–64, 66, 67, 69–74, 76, 77, 79–84, 186–249, 314–377, and 462–525 only.

5 Click **Build Selected**.

Negative current collector

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

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

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

4 On the object **fin**, select Boundaries 184, 185, 460, and 461 only.

5 Click **Build Selected**.

Positive current collector

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

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

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

4 On the object **fin**, select Boundaries 182, 183, 458, and 459 only.

5 Click **Build Selected**.

6 In the **Geometry** toolbar, click **Build All**.

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

Roller condition boundaries

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

2 In the **Settings** window for **Explicit Selection**, type `Roller condition boundaries` in the **Label** text field.

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

4 On the object **fin**, select Boundaries 85, 88, 95, 98, 105, 108, 115, 118, 125, 128, 135, 138, 145, 148, 155, 158, 174–181, 450–457, and 607–622 only.