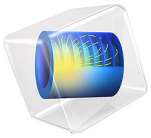


Model created in COMSOL Multiphysics 6.4

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. Instead of homogenizing the porous electrode, you can include the structural details of the porous electrodes in the model geometry. Such models are referred to as heterogeneous models. For an introduction to heterogeneous electrode modeling and homogenization, please check out the Heterogeneous NMC Electrode and Homogenizing a Heterogeneous Electrode Model examples.

This tutorial focuses on deformation and changed porosity effects when the strain induced by the lithium concentration distribution in the particles is coupled to a corresponding volumetric expansion in the Solid Mechanics interface.

In the first part of the tutorial, a unit cell model of a lithium ion-battery is set up, excluding deformation effects. The model includes electrolyte ion transport, electrode kinetics and diffusion of lithium atoms in the solid electrode particles, where the negative electrode consists of a blend of graphite and silicon. The second part of the tutorial explores the impact on the charging voltage characteristics when introducing structural mechanics to the model, including fully-coupled geometry deformation due to lithium intercalation strain. Also the local electrolyte volume fraction in the porous conductive binder and separator are affected by the local strain computed by the solid mechanics model.

Due to the usage of the Transport of Solids interface and Hyperelastic material model, the tutorial requires a Structural Mechanics Module license to run.

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 quarter spheres. In the negative electrode, the smaller spheres represent silicon, and the larger spheres graphite. On the positive side, all spheres are assumed to be made of a Nickel–Manganese–Cobalt (NMC) alloy as active material. A porous conductive binder material, containing both an electron and electrolyte conducting phase is assumed to surround the active particles in the electrodes.

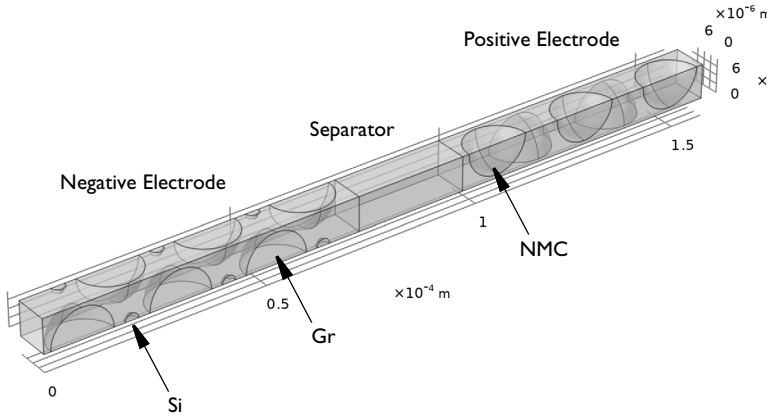


Figure 1: Model geometry. The negative graphite electrode is located toward the lower left, wherein the smaller quarter spheres define the silicon particles, and the larger quarter spheres the graphite particles, respectively. The positive electrode, containing NMC particles, is located toward the upper right.

The battery current distribution is modeled using a **Lithium-Ion Battery** interface using the **Separator** and **Porous Conductive Binder** nodes to define the concentrated battery electrolyte charge and ion transport as well as the electron conduction in the carbon filler material. Lithium diffusion in the solid electrode particles is defined using a **Transport in Solids** interface.

The charge transfer reactions occurring at the particle surfaces are defined using an **Internal Electrode Surface** node in the Lithium-Ion Battery interface. The concentration of solid lithium, solved for by the Transport in Solids interface, is coupled to the **Lithium Insertion Reaction** electrode Butler–Volmer 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 in the second part of the tutorial using a **Solid Mechanics** interface, where the expansion is defined using an **Intercalation Strain** node (subnode to the **Linear-Elastic Material** node). The strain is defined as a function of the local solid lithium concentration using an interpolation function, based on experimental data (Ref. 1).

Silicon expands up to 300% upon full lithiation. As a result of these large deforrmations, a linear material model has limited validity in the surrounding binder around the silicon particles. For this reason, a **Hyperelastic** material model for the binder in the negative electrode is used.

FRAME OF REFERENCE AND THE SOLID LITHIUM CONCENTRATION

In COMSOL Multiphysics, the partial differential equations of physics interfaces are usually formulated either in a **Spatial** frame (coordinate system), with coordinate axes fixed in space, or in a **Material** frame, fixed to the material in its reference configuration, following the material as it deforms. (The former is often referred to as an *Eulerian* formulation, while the latter is a *Lagrangian* formulation.)

Most equations and variables in the battery interfaces are defined with reference to the spatial frame (except the particle intercalation concentration in porous electrode nodes). In most battery models however, the spatial and material frames are identical, and no consideration with regards to frame handling needs to be taken.

In this tutorial however, due to the large deformation of the silicon particles, we induce a split between the material and spatial frame (this is performed by having **Include Geometric Nonlinearity** enabled in the time-dependent solver, which deforms the mesh and spatial frame according to the deformations computed by the solid mechanics interface). As a result of this, certain care needs to be taken when considering the concentration values computed by the mass balance equations in the solid particles.

The equilibrium potential functions used for defining the electrode reactions in the Battery Design material library are defined as functions of concentrations in the reference **Material** frame, that is, for a control volume excluding material strains induced by lithium

intercalation. This means that any concentration value we use for evaluation of the local electrode equilibrium potential needs to be defined with reference to the material frame.

One option to do this is to use the **Solid** node in the **Transport of Diluted Species** interface (which solves for the material balance on the spatial frame), and then use one of the built-in transformation variables (such as `spatial.detInvF`) for converting the spatial concentration variables to the corresponding values for the material frame. In this tutorial we however choose to use the **Transport of Solids** interface, since this physics interface defines its material balance directly on the material frame, resulting in a reduced number of numerical operations.

To read more about frame handling, check out the *Deformed Mesh Fundamentals* section in the COMSOL Multiphysics Reference Manual.

CHANGED ELECTROLYTE VOLUME FRACTIONS DUE TO INTERCALATION STRAIN

In part two of the tutorial, the local volumetric strain ε is computed by the solid mechanics model. In the porous conductive binder and separator domains, which are blended materials, comprising both a solid (conducting or nonconducting) and an electrolyte phase, it is assumed that all volumetric strain is accommodated by a changed porosity, treating the solid part of the blend as incompressible.

The electrolyte volume fraction (porosity) is hence defined as

$$\varepsilon_l = \frac{\varepsilon_{l,\,\mathrm{ref}} + \varepsilon}{\varepsilon_{s,\,\mathrm{ref}} + \varepsilon_{l,\,\mathrm{ref}} + \varepsilon} = \frac{\varepsilon_{l,\,\mathrm{ref}} + \varepsilon}{1 + \varepsilon} = 1 - \frac{\varepsilon_{s,\,\mathrm{ref}}}{1 + \varepsilon} \tag{1}$$

where $\varepsilon_{l,\mathrm{ref}}$ and $\varepsilon_{s,\mathrm{ref}}$ are the nondeformed electrolyte and solid volume fractions, respectively, fulfilling the relation $\varepsilon_{s,\mathrm{ref}} + \varepsilon_{l,\mathrm{ref}} = 1$.

In continuation, effective transport parameters for electrolyte conductivity and diffusivity of the electrolyte salt are defined as

$$\sigma_{l,\,\mathrm{eff}} = \varepsilon_l^{3/2}\sigma_l \tag{2}$$

and

$$D_{l,\,\mathrm{eff}} = \varepsilon_l^{3/2} D_l \tag{3}$$

where σ_l and D_l are the bulk conductivity and diffusivity values, respectively.

STUDIES

Two separate studies, both simulating a 1 h charge from 0 to 100% state of charge, are used in the tutorial. The first study excludes structural mechanic effects, whereas the second includes fully two-way solid mechanics-electrochemistry couplings. **Automatic remeshing** is enabled in the second study in order avoid inverted mesh elements due to deformation of the computational mesh.

Results and Discussion

Figure 2 shows the relative lithiation levels in the particles after 6 min for the fully coupled model. All particles exhibit solid concentration gradients in the radial direction. This early into the charge cycle, the silicon particles have already been lithiated to almost 60%, whereas the graphite has only been lithiated to levels below 10%. This indicates that the silicon material in the electrode will mainly be utilized when operating the battery at low state-of-charge levels. (For a deeper discussion on the behavior of blended graphite-silicon electrodes, see the Silicon–Graphite-Blended Electrode with Thermodynamic Voltage Hysteresis example).

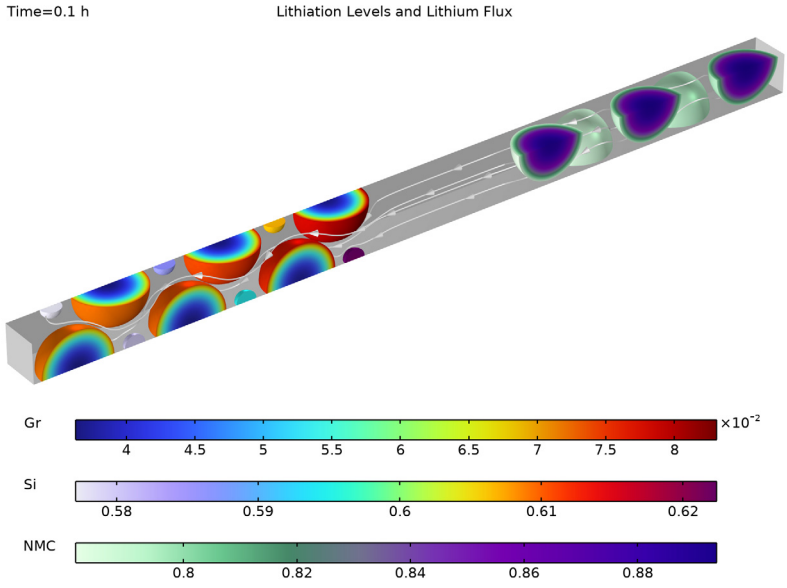


Figure 2: Relative lithiation levels in the electrode particles at t = 6 min.

Figure 3 shows the same plot at the end of the 1 h charge, with added black edges to indicate the original, nondeformed, geometry. Due to the intercalation strain, the negative electrode has expanded somewhat.

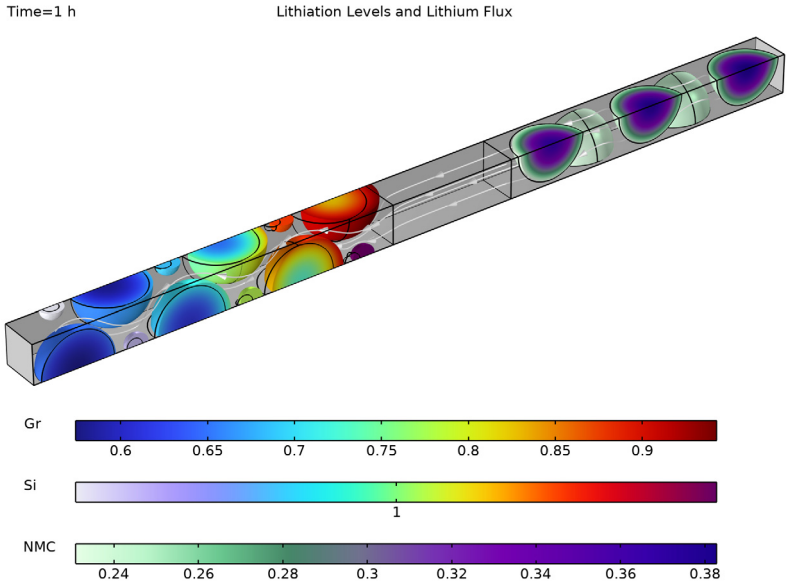


Figure 3: Relative lithiation levels in the electrode particles at t = 1 h. The black edges indicate the shape of the original (nondeformed) geometry.

Figure 4 compares the charging voltage curves for the two models. The curves are nearly identical, indicating that including the two-way coupling to solid mechanics has limited impact on the electrochemical model.

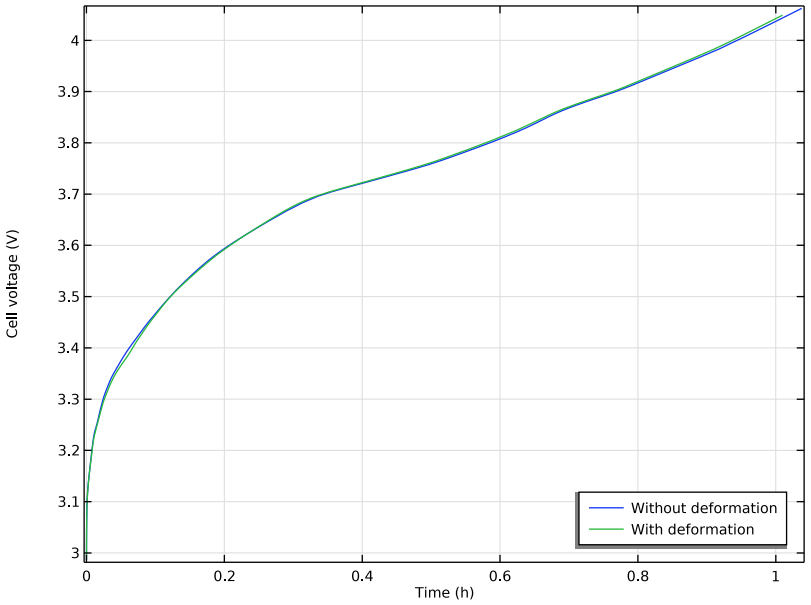


Figure 4: Charging voltage for the two models.

Finally, the average outward normal stress on the positive current collector boundary is plotted in Figure 5. The dominating features of the plot are governed by the intercalation strain function of graphite.

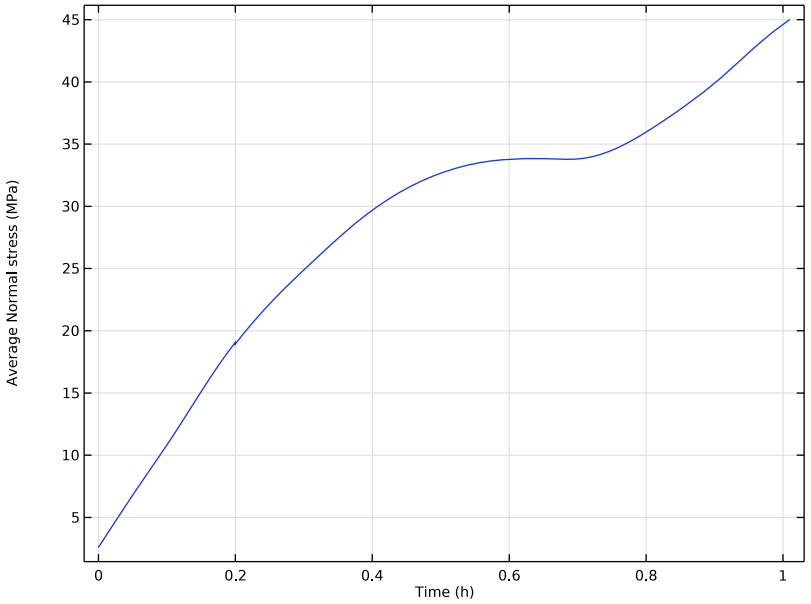


Figure 5: Average outward normal stress on the positive current collector boundary.

Reference

1. J.B. Siegel, A.G. Stefanopoulou, P. Hagans, Y. Ding, and D. Gorsich, "Expansion of Lithium Ion Pouch Cell Batteries: Observations from Neutron Imaging," *J. Electrochemical Soc.*, vol. 160, p. A1031, 2013.

Application Library path: `Battery_Design_Module/Heterogeneous_Models/heterogeneous_lib`

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 **Chemical Species Transport** > **Transport in Solids (ts)**.

3 Click **Add**.

4 In the **Select Physics** tree, select **Electrochemistry** > **Batteries** > **Lithium-Ion Battery (liion)**.

5 Click **Add**.

6 Click **Study**.

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

8 Click **Done**.

GEOMETRY 1

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_lib_geom_sequence.mph`.

3 In the **Insert Sequence** dialog, select **Geometry 1** in the **Select geometry sequence to insert** list.

4 Click **OK**.

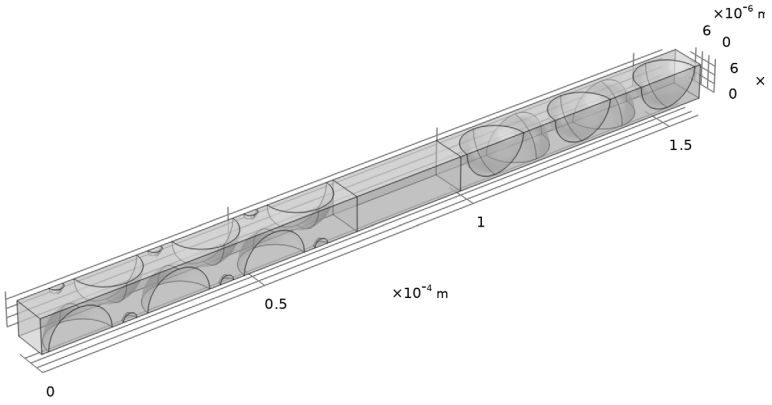
5 In the **Geometry** toolbar, click **Build All**.

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

7 Click the **Show Axis Orientation** button in the **Graphics** toolbar.

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

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



10 In the **Model Builder** window, collapse the **Geometry 1** node.

GLOBAL DEFINITIONS

Geometry Parameters

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

2 In the **Settings** window for **Parameters**, type `Geometry Parameters` in the **Label** text field.

Physics Parameters

1 In the **Home** toolbar, click **Parameters** and choose **Add** > **Parameters**.

2 In the **Settings** window for **Parameters**, type `Physics Parameters` in the **Label** text field.

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

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

ADD MATERIAL

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

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

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

4 Right-click and choose **Add to Component 1 (comp1)**.

5 In the tree, select **Battery** > **Electrodes** > **Silicon, LixSi (Negative, Li-ion Battery)**.

6 Right-click and choose **Add to Component 1 (comp1)**.

7 In the tree, select **Battery** > **Electrodes** > **NMC 111, LiNi0.33Mn0.33Co0.33O2 (Positive, Li-ion Battery)**.

8 Right-click and choose **Add to Component 1 (comp1)**.

9 In the tree, select **Battery** > **Electrolytes** > **LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery)**.

10 Right-click and choose **Add to Component 1 (comp1)**.

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

MATERIALS

Graphite, LixC6 MCMB (Negative, Li-ion Battery) (mat1)

Set the correct domain selection of the graphite material that you just added.

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

2 From the **Selection** list, choose **Graphite Particles**.

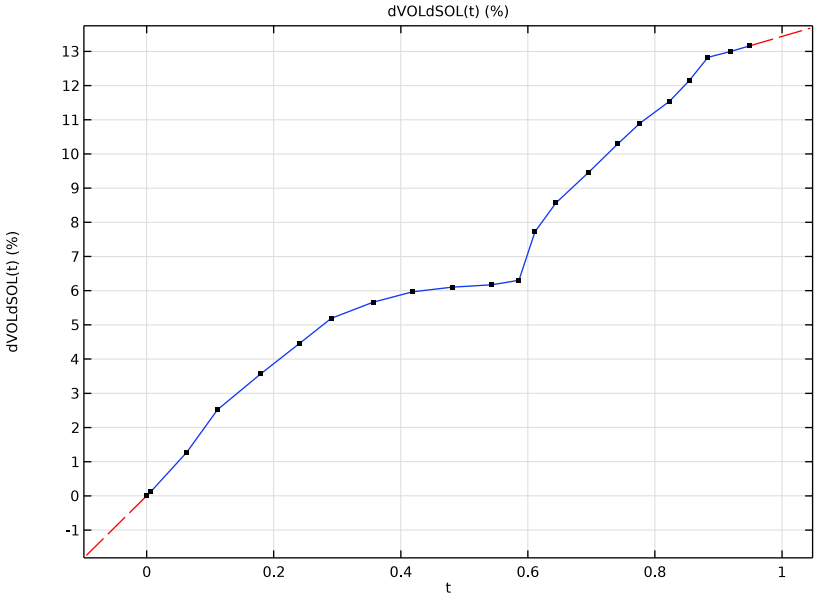
3 In the **Model Builder** window, expand the **Graphite, LixC6 MCMB (Negative, Li-ion Battery) (mat1)** node.

The electrode material nodes define the material strain as a function of the lithium intercalation level. You can view the strain function for graphite as follows:

Interpolation 1 (dVOLdSOL)

1 In the **Model Builder** window, expand the **Component 1 (comp1)** > **Materials** > **Graphite, LixC6 MCMB (Negative, Li-ion Battery) (mat1)** > **Intercalation strain (is)** node, then click **Interpolation 1 (dVOLdSOL)**.

2 In the **Settings** window for **Interpolation**, click **Plot**.



MATERIALS

Graphite, LixC6 MCMB (Negative, Li-ion Battery) (mat1)

In the **Model Builder** window, collapse the **Component 1 (comp1)** > **Materials** > **Graphite, LixC6 MCMB (Negative, Li-ion Battery) (mat1)** node.

Silicon, LixSi (Negative, Li-ion Battery) (mat2)

1 In the **Model Builder** window, click **Silicon, LixSi (Negative, Li-ion Battery) (mat2)**.

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

3 From the **Selection** list, choose **Silicon Particles**.

NMC 111, LiNi0.33Mn0.33Co0.33O2 (Positive, Li-ion Battery) (mat3)

1 In the **Model Builder** window, click **NMC 111, LiNi0.33Mn0.33Co0.33O2 (Positive, Li-ion Battery) (mat3)**.

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

3 From the **Selection** list, choose **NMC Particles**.

LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery) (mat4)

1 In the **Model Builder** window, click **LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery) (mat4)**.

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

3 From the **Selection** list, choose **Electrolyte Domains**.

Duplicate the electrode materials and change the selections of the duplicates to make the material properties available also at the particle surfaces. These properties will be used when defining the electrode reactions.

Graphite, LixC6 MCMB (Negative, Li-ion Battery) 1 (mat5)

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Materials** right-click **Graphite, LixC6 MCMB (Negative, Li-ion Battery) (mat1)** and choose **Duplicate**.

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

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

4 From the **Selection** list, choose **Graphite Electrode Particle Surfaces**.

Silicon, LixSi (Negative, Li-ion Battery) 1 (mat6)

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Materials** right-click **Silicon, LixSi (Negative, Li-ion Battery) (mat2)** and choose **Duplicate**.

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

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

4 From the **Selection** list, choose **Si Particle Surfaces**.

NMC 111, LiNi0.33Mn0.33Co0.33O2 (Positive, Li-ion Battery) 1 (mat7)

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Materials** right-click **NMC 111, LiNi0.33Mn0.33Co0.33O2 (Positive, Li-ion Battery) (mat3)** and choose **Duplicate**.

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

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

4 From the **Selection** list, choose **NMC Electrode Particle Surfaces**.

LITHIUM-ION BATTERY (LIION)

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

2 In the **Settings** window for **Lithium-Ion Battery**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Electrolyte Domains**.

Lower the discretization order of the lithium-ion battery interface. This will reduce the computational load.

4 Click to expand the **Discretization** section. From the **Electrolyte potential** list, choose **Linear**.

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

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

Separator 1

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

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

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

Porous Conductive Binder 1

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

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

3 From the **Selection** list, choose **Porous Conductive Binder**.

4 Locate the **Conductive Binder Properties** section. In the σ_s text field, type `sigmas_pb`.

5 Locate the **Porous Matrix Properties** section. In the ε_s text field, type `1-epsl_ref_pb`.

6 In the ε_l text field, type `epsl_ref_pb`.

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

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 **Particle Surfaces**.

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 In the c text field, type `c`.

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

5 In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0_ref`.

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. From the list, choose **Average current density**.

5 In the $i_{s,average}$ text field, type `i_app`.

TRANSPORT IN SOLIDS (TS)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Transport in Solids (ts)**.

2 In the **Settings** window for **Transport in Solids**, locate the **Domain Selection** section.

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

Solid - Graphite

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Transport in Solids (ts)** click **Solid 1**.

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

3 Locate the **Diffusion** section. From the **Material** list, choose **Graphite, LixC6 MCMB (Negative, Li-ion Battery) (mat1)**.

4 From the D_c list, choose **Basic (def)**.

Solid - Silicon

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

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

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

4 Locate the **Diffusion** section. From the **Material** list, choose **Silicon, LixSi (Negative, Li-ion Battery) (mat2)**.

5 From the D_c list, choose **Basic (def)**.

Solid - NMC

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

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

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

4 Locate the **Diffusion** section. From the **Material** list, choose **NMC 111, LiNi0.33Mn0.33Co0.33O2 (Positive, Li-ion Battery) (mat3)**.

5 From the D_c list, choose **Basic (def)**.

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 **Particle Surfaces**.

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

5 In the n text field, type `1`.

6 In the ν_c text field, type `1`.

Initial Values 2

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

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

3 From the **Selection** list, choose **Graphite Particles**.

4 Locate the **Initial Values** section. In the c text field, type `cs0_Gr`.

Initial Values 3

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 **Silicon Particles**.

4 Locate the **Initial Values** section. In the c text field, type `cs0_Si`.

Initial Values 1

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 c text field, type `cs0_pos`.

MESH 1

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

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

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

4 In the **Mesh** toolbar, click **Clear Sequence**.

Free Tetrahedral 1

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

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 **Geometric entity level** list, choose **Domain**.

4 From the **Selection** list, choose **Silicon Particles**.

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

Size

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

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

3 Click the **Custom** button.

4 Locate the **Element Size Parameters** section. In the **Maximum element size** text field, type `s_unit_cell/3`.

5 In the **Minimum element size** text field, type `s_gap/4`.

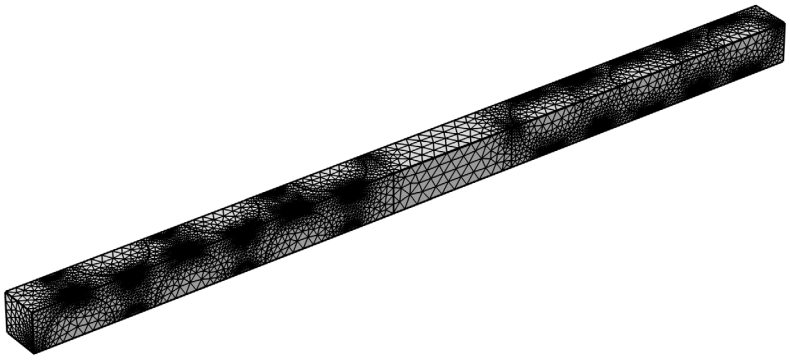
6 In the **Maximum element growth rate** text field, type `1.3`.

7 In the **Resolution of narrow regions** text field, type `2.5`.

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

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

10 Click the **Show Grid** button in the **Graphics** toolbar.



DEFINITIONS

Global Variable Probe 1 (var1)

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

2 In the **Settings** window for **Global Variable Probe**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)** > **Lithium-Ion Battery** > **liion.phis0_ec1 - Electric potential on boundary - V**.

3 Locate the **Expression** section.

4 Select the **Description** checkbox. In the associated text field, type `Cell voltage`.

STUDY 1

Step 2: Time Dependent

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

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

3 From the **Time unit** list, choose **h**.

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

5 In the **Settings** window for **Study**, locate the **Study Settings** section.

6 Clear the **Generate default plots** checkbox.

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

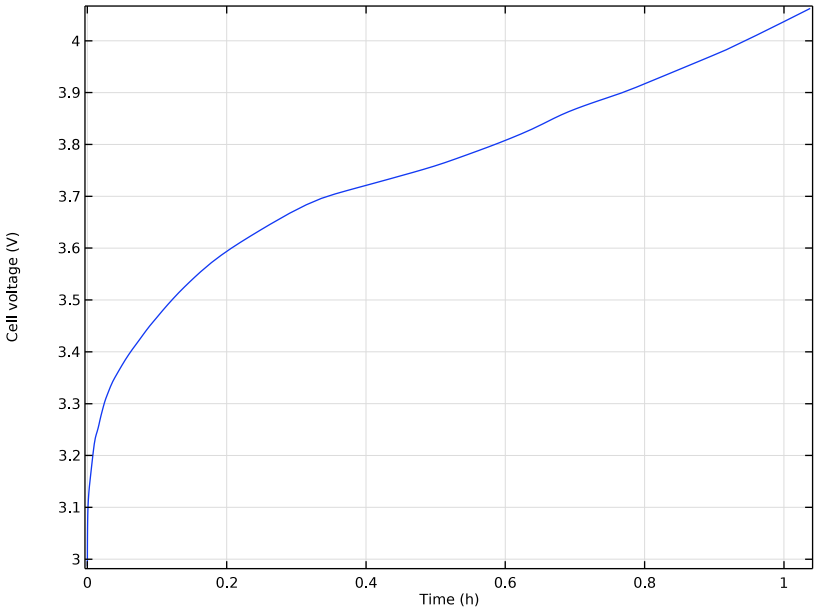
RESULTS

Cell Voltage vs. Time

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

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

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



Lithiation Levels and Lithium Flux

1 In the **Results** toolbar, click **3D Plot Group**.

2 In the **Settings** window for **3D Plot Group**, type `Lithiation Levels and Lithium Flux` in the **Label** text field.

3 Click to expand the **Title** section. From the **Title type** list, choose **Label**.

4 Locate the **Plot Settings** section. Clear the **Plot dataset edges** checkbox.

5 Locate the **Color Legend** section. Select the **Show titles** checkbox.

6 From the **Position** list, choose **Bottom**.

Volume 1

1 Right-click **Lithiation Levels and Lithium Flux** and choose **Volume**.

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

3 In the **Expression** text field, type `c/csmax_Gr`.

4 Locate the **Coloring and Style** section. In the **Color legend title** text field, type `Gr`.

Selection 1

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

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

3 From the **Selection** list, choose **Graphite Particles**.

Volume 2

1 In the **Model Builder** window, under **Results** > **Lithiation Levels and Lithium Flux** right-click **Volume 1** and choose **Duplicate**.

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

3 In the **Expression** text field, type `c/csmax_Si`.

4 Locate the **Coloring and Style** section. From the **Color table** list, choose **Prism**.

5 In the **Color legend title** text field, type `Si`.

Selection 1

1 In the **Model Builder** window, expand the **Volume 2** node, then click **Selection 1**.

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

3 From the **Selection** list, choose **Silicon Particles**.

Volume 3

1 In the **Model Builder** window, under **Results** > **Lithiation Levels and Lithium Flux** right-click **Volume 2** and choose **Duplicate**.

2 In the **Model Builder** window, click **Volume 3**.

3 In the **Settings** window for **Volume**, locate the **Expression** section.

4 In the **Expression** text field, type `c/csmax_pos`.

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

6 In the **Color legend title** text field, type `NMC`.

Selection 1

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

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

3 From the **Selection** list, choose **NMC Particles**.

4 In the **Lithiation Levels and Lithium Flux** toolbar, click **Plot**.

Streamline 1

1 In the **Model Builder** window, right-click **Lithiation Levels and Lithium Flux** and choose **Streamline**.

2 In the **Settings** window for **Streamline**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)** > **Lithium-Ion Battery** > **liion.Nposx,...,liion.Nposz - Positive ion flux**.

3 Locate the **Streamline Positioning** section. In the **Number** text field, type 4.

4 Select Boundary 59 only.

5 Locate the **Coloring and Style** section. Find the **Point style** subsection. From the **Type** list, choose **Arrow**.

6 From the **Arrow distribution** list, choose **Equal inverse time**.

7 From the **Color** list, choose **White**.

Surface 1

1 Right-click **Lithiation Levels and Lithium Flux** and choose **Surface**.

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

3 In the **Expression** text field, type 1.

4 Locate the **Coloring and Style** section. From the **Coloring** list, choose **Uniform**.

5 From the **Color** list, choose **Gray**.

Selection 1

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

2 Select Boundaries 1, 3, 5, 56, 58, 61, 63, and 84 only.

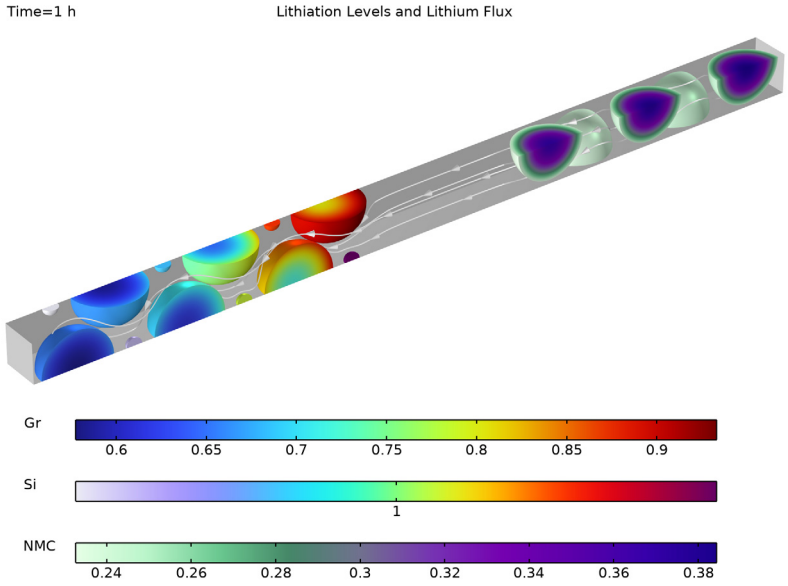
3 In the **Lithiation Levels and Lithium Flux** toolbar, click **Plot**.

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

Lithiation Levels and Lithium Flux

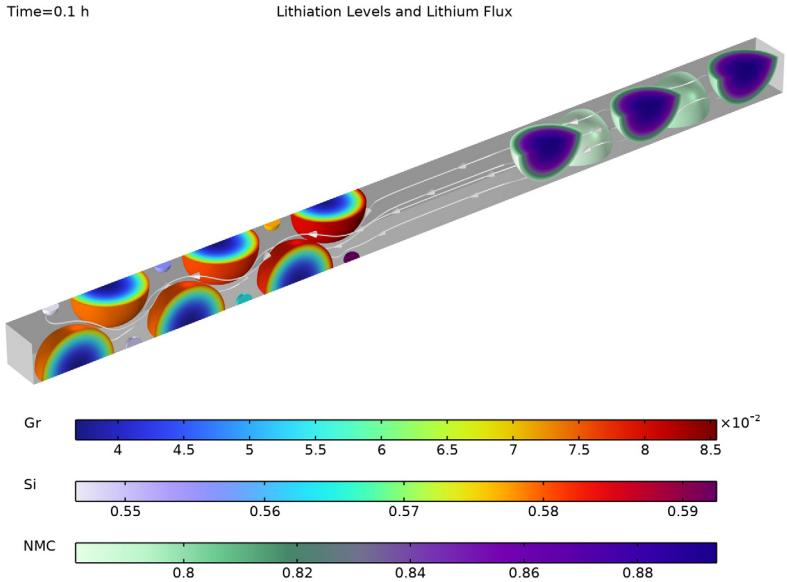
1 In the **Model Builder** window, under **Results** click **Lithiation Levels and Lithium Flux**.

2 In the **Lithiation Levels and Lithium Flux** toolbar, click **Plot**.



3 In the **Settings** window for **3D Plot Group**, locate the **Data** section.

4 From the **Time (h)** list, choose **0.1**.



Animation 1

1 In the **Results** toolbar, click **Animation** and choose **Player**.

2 In the **Settings** window for **Animation**, locate the **Scene** section.

3 From the **Subject** list, choose **Lithiation Levels and Lithium Flux**.

4 Locate the **Frames** section. From the **Frame selection** list, choose **All**.

5 Locate the **Playing** section. In the **Display each frame for** text field, type `0.5`.

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

COMPONENT 1 (COMP1)

Now extend the model to include structural-mechanics effects due to expansion/contraction of the electrode particles upon lithium intercalation/deintercalation.

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 the **Add to Component 1** button in the window toolbar.

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

SOLID MECHANICS (SOLID)

Due to the slow intercalation processes, mechanical wave propagation can be ignored in the model; set the transient behavior to **Quasistatic**.

1 In the **Settings** window for **Solid Mechanics**, locate the **Structural Transient Behavior** section.

2 From the list, choose **Quasistatic**.

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 **Linear Elastic Material** section.

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

4 From the ν list, choose **User defined**. In the associated text field, type `nu_pb`.

5 From the ρ list, choose **User defined**. In the associated text field, type `rho`.

Linear Elastic Material 2

1 In the **Physics** toolbar, click **Domains** and choose **Linear Elastic Material**.

2 In the **Settings** window for **Linear Elastic Material**, locate the **Domain Selection** section.

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

4 Locate the **Model Input** section. In the c text field, type `c`.

Intercalation Strain 1

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

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

3 In the c text field, type `c`.

Linear Elastic Material 3

1 In the **Physics** toolbar, click **Domains** and choose **Linear Elastic Material**.

2 In the **Settings** window for **Linear Elastic Material**, locate the **Domain Selection** section.

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

4 Locate the **Linear Elastic Material** section. From the E list, choose **User defined**. In the associated text field, type `E_sep`.

5 From the ν list, choose **User defined**. In the associated text field, type `nu_sep`.

6 From the ρ list, choose **User defined**. In the associated text field, type `rho`.

Hyperelastic Material 1

Due to the presence of silicon in the negative electrode, very large deformations (up to 300%) are expected, which, in turn, are not well described by a linear material model. Therefore, change the model to **Hyperelastic** in the negative electrode as follows:

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

2 Select Domain 1 only.

3 In the **Settings** window for **Hyperelastic Material**, locate the **Hyperelastic Material** section.

4 From the **Specify** list, choose **Young's modulus and Poisson's ratio**.

5 From the *E* list, choose **User defined**. In the associated text field, type `E_pb`.

6 From the ν list, choose **User defined**. In the associated text field, type `nu_pb`.

7 From the ρ list, choose **User defined**. In the associated text field, type `rho`.

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 **Symmetry boundaries**.

Fixed Constraint 1

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

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

3 From the **Selection** list, choose **Current Collectors**.

MATERIALS

Silicon, LixSi (Negative, Li-ion Battery) (mat2)

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Materials** click **Silicon, LixSi (Negative, Li-ion Battery) (mat2)**.

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

3 In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Young's modulus	E	`150[GPa]`	Pa	Young's modulus and Poisson's ratio
Poisson's ratio	nu	`0.3`	1	Young's modulus and Poisson's ratio

NMC 111, LiNi0.33Mn0.33Co0.33O2 (Positive, Li-ion Battery) (mat3)

1 In the **Model Builder** window, click **NMC 111, LiNi0.33Mn0.33Co0.33O2 (Positive, Li-ion Battery) (mat3)**.

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

3 In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Density	rho	1000	kg/m³	Basic

DEFINITIONS

As a result of the material strain, the porosity (that is, the electrolyte volume fraction) will no longer be constant in the separator and porous conductive binder domains. Add variables for the electrolyte volume fractions as functions of the strain as follows:

Variables - Separator

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Definitions** and choose **Variables**.

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

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

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

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

Name	Expression	Unit	Description
eps_solid	(1-epsl_ref_sep)/(1+solid.evol)		Solid (nonelectrolyte) volume fraction in deformed geometry
epsl	max(1-eps_solid, 0.01)		Electrolyte volume fraction in deformed geometry

Variables - Porous Conductive Binder

1 Right-click **Variables - Separator** and choose **Duplicate**.

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

3 Locate the **Geometric Entity Selection** section. From the **Selection** list, choose **Porous Conductive Binder**.

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

Name	Expression	Unit	Description
eps_solid	(1-epsl_ref_pb)/(1+solid.evol)		Solid (nonelectrolyte) volume fraction in deformed geometry

LITHIUM-ION BATTERY (LIION)

Separator 1

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

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

3 In the ε_l text field, type `epsl`.

Porous Conductive Binder 1

1 In the **Model Builder** window, click **Porous Conductive Binder 1**.

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

3 In the ε_s text field, type `eps_solid`.

4 In the ε_l text field, type `epsl`.

ADD STUDY

The modified model is now ready for solving. Add a second study to solve for the new model, and modify the settings of the first study to solve for the nonstructural mechanics model as follows:

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

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

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

4 Right-click and choose **Add Study**.

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

DEFINITIONS

Global Variable Probe 2 (var2)

Create a new cell voltage probe for the second study. In this way, the probe table values of Study 1 will not be overwritten by Study 2.

1. In the **Model Builder** window, under **Component 1 (comp1)** > **Definitions** right-click **Global Variable Probe 1 (var1)** and choose **Duplicate**.
2. In the **Settings** window for **Global Variable Probe**, click to expand the **Table and Window Settings** section.
3. Click + **Add Table**.

Boundary Probe 1 (bnd1)

Also create a probe for the normal stress at the positive current collector to be used in the second study.

1. In the **Definitions** toolbar, click  **Probes** and choose **Boundary Probe**.
2. In the **Settings** window for **Boundary Probe**, locate the **Source Selection** section.
3. From the **Selection** list, choose **Positive Current Collector**.
4. Click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)** > **Solid Mechanics** > **Stress** > **solid.stn - Normal stress - N/m²**.
5. Locate the **Expression** section. In the **Expression** text field, type `-solid.stn`.
6. From the **Table and plot unit** list, choose **MPa**.
7. Click to expand the **Table and Window Settings** section. Click + **Add Table**.
8. Click + **Add Plot Window**.

STUDY 1 - EXCLUDING SOLID MECHANICS

1. In the **Model Builder** window, click **Study 1**.
2. In the **Settings** window for **Study**, type `Study 1 - Excluding Solid Mechanics` in the **Label** text field.

Step 2: Time Dependent

1. In the **Model Builder** window, under **Study 1 - Excluding Solid Mechanics** click **Step 2: Time Dependent**.
2. In the **Settings** window for **Time Dependent**, locate the **Physics and Variables Selection** section.

3 In the **Solve for** column of the table, under **Component 1 (comp1)**, clear the checkbox for **Solid Mechanics (solid)**.

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

5 In the **Probes** list box, select **Global Variable Probe 2 (var2)**.

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

7 In the **Probes** list box, select **Boundary Probe 1 (bnd1)**.

8 Under **Probes**, click **Delete**.

STUDY 2 - FULL MODEL

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

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

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

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

3 From the **Time unit** list, choose **h**.

4 Locate the **Results While Solving** section. From the **Probes** list, choose **Manual**.

5 In the **Probes** list box, select **Global Variable Probe 1 (var1)**.

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

Note that by adding the **Hyperelastic Material** node under **Solid Mechanics**, the **Include geometric nonlinearity** checkbox is enabled by default, and cannot be cleared. **Include geometric nonlinearity** will displace the computational mesh according to the strain computed by the **Solid Mechanics** interface.

7 Click to expand the **Study Extensions** section. Enable automatic remeshing to make sure that the computational mesh does not get compromised as a result of the displacement.

8 Select the **Automatic remeshing** checkbox.

Solution 3 (sol3)

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

2 In the **Model Builder** window, expand the **Solution 3 (sol3)** node.

Add a user-defined remeshing condition that performs a remeshing operation if the relative volume of an element shrinks by more than 50%.

3 In the **Model Builder** window, expand the **Study 2 - Full Model** > **Solver Configurations** > **Solution 3 (sol3)** > **Time-Dependent Solver 1** node, then click **Automatic Remeshing**.

4 In the **Settings** window for **Automatic Remeshing**, locate the **Condition for Remeshing** section.

5 In the **Mesh quality expression** text field, type `comp1.spatial.relVolMin`.

6 In the **Stop when mesh quality is below** text field, type `0.5`.

7 Locate the **Remesh** section. From the **Consistent initialization** list, choose **On**.

To increase the robustness of the solver when using **Automatic remeshing**, change the Jacobian update to **Once per timestep**. This improves convergence.

8 In the **Model Builder** window, expand the **Study 2 - Full Model** > **Solver Configurations** > **Solution 3 (sol3)** > **Time-Dependent Solver 1** > **Segregated 1** node, then click **Solid Mechanics**.

9 In the **Settings** window for **Segregated Step**, click to expand the **Method and Termination** section.

10 From the **Jacobian update** list, choose **Once per time step**.

11 In the **Model Builder** window, under **Study 2 - Full Model** > **Solver Configurations** > **Solution 3 (sol3)** > **Time-Dependent Solver 1** > **Segregated 1** click **Transport in Solids**.

12 In the **Settings** window for **Segregated Step**, locate the **Method and Termination** section.

13 From the **Jacobian update** list, choose **Once per time step**.

14 In the **Model Builder** window, click **Study 2 - Full Model**.

15 In the **Settings** window for **Study**, locate the **Study Settings** section.

16 Clear the **Generate default plots** checkbox.

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

RESULTS

Cell Voltage vs. Time

1 In the **Model Builder** window, expand the **Results** > **Cell Voltage vs. Time** node, then click **Cell Voltage vs. Time**.

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

3 Select the **Show legends** checkbox.

Probe Table Graph 1

1 In the **Model Builder** window, click **Probe Table Graph 1**.

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

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

4 In the table, enter the following settings:

Legends
Without deformation

Probe Table Graph 2

1 In the **Model Builder** window, click **Probe Table Graph 2**.

2 In the **Settings** window for **Table Graph**, locate the **Legends** section.

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

4 In the table, enter the following settings:

Legends
With deformation

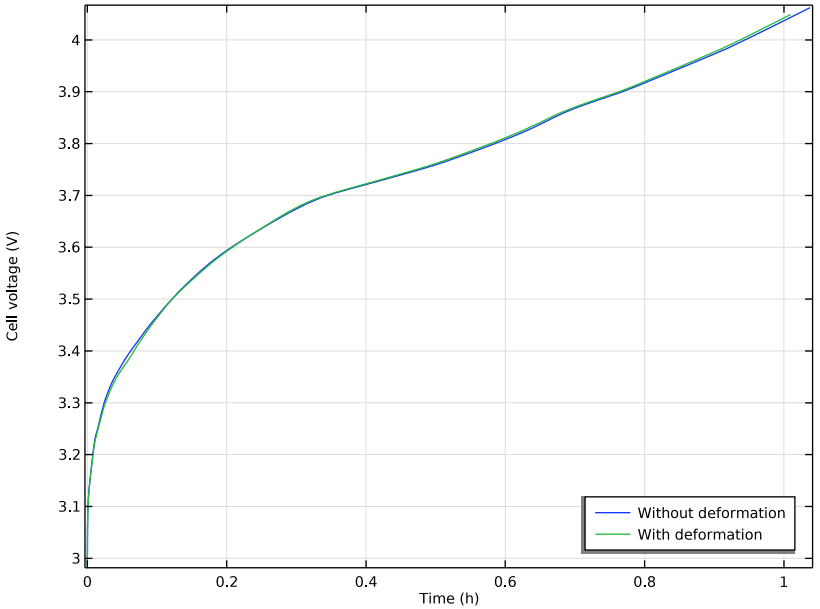
Cell Voltage vs. Time

1 In the **Model Builder** window, click **Cell Voltage vs. Time**.

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

3 From the **Position** list, choose **Lower right**.

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



Study 2 - Full Model/Remeshed Solution 1 (sol5)

1 In the **Model Builder** window, expand the **Results** > **Datasets** node, then click **Study 2 - Full Model/Remeshed Solution 1 (sol5)**.

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

3 From the **Frame** list, choose **Spatial (x, y, z)**.

Lithiation Levels and Lithium Flux

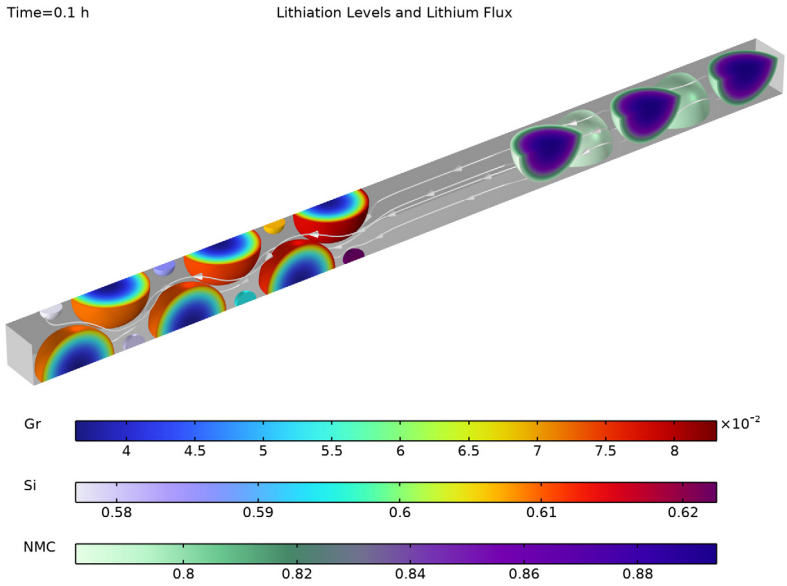
1 In the **Model Builder** window, under **Results** click **Lithiation Levels and Lithium Flux**.

2 In the **Settings** window for **3D Plot Group**, locate the **Data** section.

3 From the **Dataset** list, choose **Study 2 - Full Model/Remeshed Solution 1 (sol5)**.

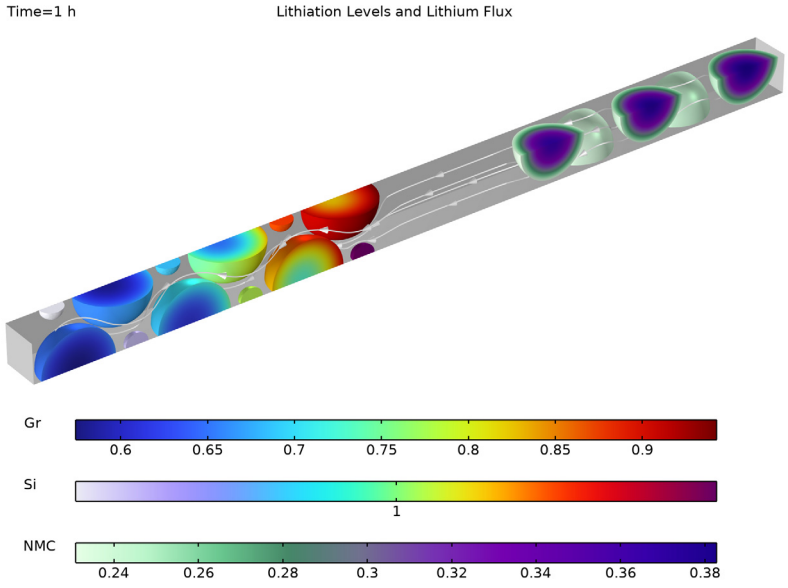
4 From the **Time (h)** list, choose **Interpolation**.

5 In the **Lithiation Levels and Lithium Flux** toolbar, click **Plot**.



6 From the **Time (h)** list, choose **Last (1)**.

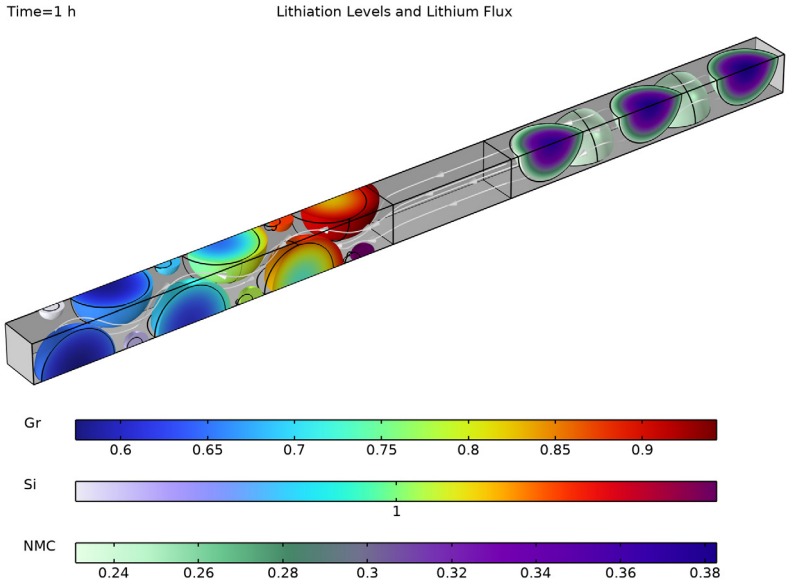
7 In the **Lithiation Levels and Lithium Flux** toolbar, click **Plot**.



Enable the data set edges to compare the deformed geometry with the nondeformed geometry.

8 Locate the **Plot Settings** section. Select the **Plot dataset edges** checkbox.

9 In the **Lithiation Levels and Lithium Flux** toolbar, click **Plot**.



10 Clear the **Plot dataset edges** checkbox.

Current Collector Normal Stress vs. Time

1 In the **Model Builder** window, under **Results** click **Probe Plot Group 3**.

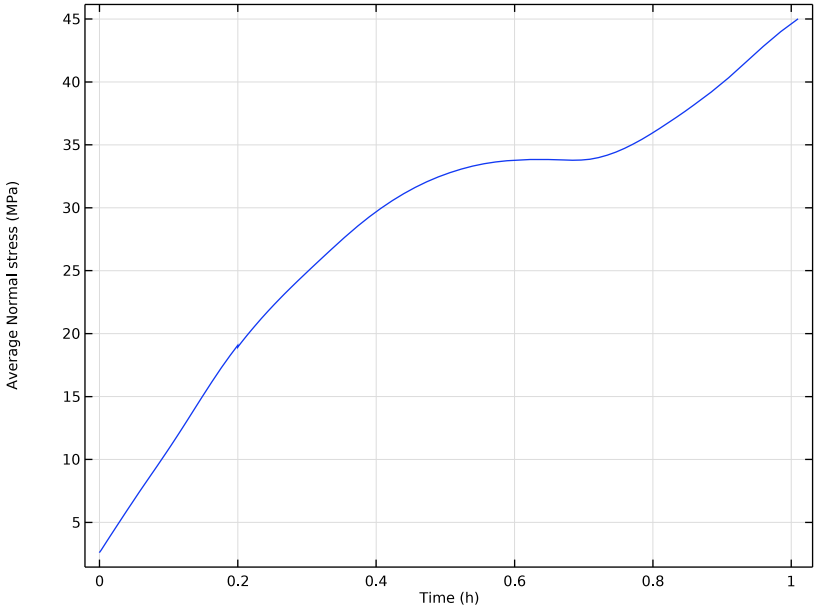
2 In the **Settings** window for **1D Plot Group**, type `Current Collector Normal Stress vs. Time` in the **Label** text field.

3 Locate the **Plot Settings** section.

4 Select the **y-axis label** checkbox. In the associated text field, type `Average Normal stress (MPa)`.

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

6 In the **Current Collector Normal Stress vs. Time** toolbar, click **Plot**.



Animation 1

1 In the **Model Builder** window, under **Results** > **Export** click **Animation 1**.

2 In the **Settings** window for **Animation**, locate the **Animation Editing** section.

3 From the **Time selection** list, choose **Interpolated**.

4 In the **Times (h)** text field, type `range(0,0.1,1)`.

5 Click the **Play** button in the **Graphics** toolbar.