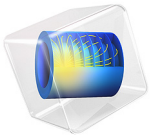


Heterogeneous NMC Electrode

Introduction

In this example, time-dependent discharge and electrochemical impedance spectroscopy (EIS) simulations are made on a heterogeneous NMC (Nickel-Manganese-Cobalt) electrode structure.

A solid mechanics simulation is also made to study the effect of electrode expansion/ contraction on the particle and binder stresses.

Model Definition

The model geometry is heterogeneous with regards to the electrode particles. However, since carbon filler, binder, and electrolyte are treated as a single porous conductive binder domain following a partly homogenized approach as described in Ref. 1.

Figure 1 shows the model geometry which is generated from tomography data (Ref. 2) using a Model Method. The geometry consists of one separator domain, one domain representing the porous conductive binder, and number of particle domains. How the geometry is created is documented in the Heterogeneous Electrode Geometry Generation tutorial.

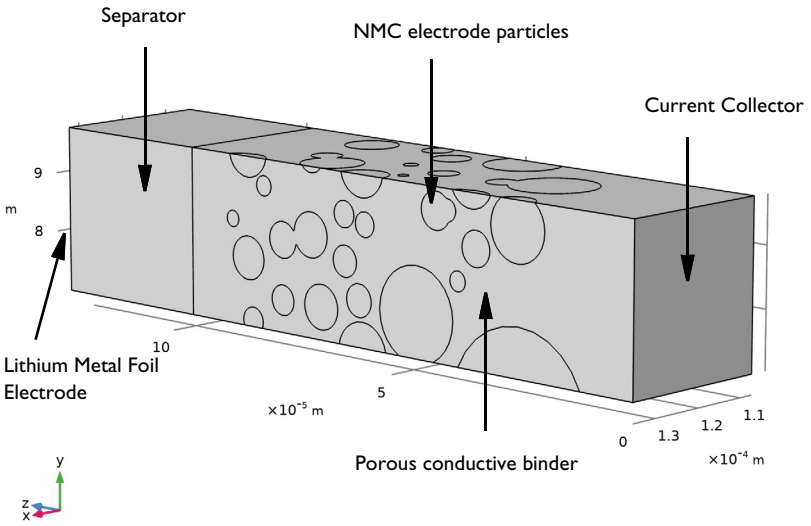


Figure 1: Model geometry.

BATTERY MODEL

The **Lithium-Ion Battery** interface is used to define the electrolyte mass and charge transport, as well as the charge transport of the electrode phase, using the Battery Material Library materials **NMC 111, LiNi0.33Mn0.33Co0.33O2**, **Lithium Metal, Li**, and **LiPF6 in 3:7 EC:EMC** to define the electrode and electrolyte properties, respectively.

The **Transport of Diluted Species** interface is used to define the diffusion of intercalated lithium within the electrode particles.

The electrochemically active electrolyte-electrode interfaces at the particle surfaces and the negative lithium foil electrode are defined using the **Electrode Surface** nodes in the Lithium-Ion Battery interface, using **Electrode Reaction** child-nodes to define the electrode kinetics. The surface intercalation flux of lithium at the particle surfaces are coupled to the electrochemical reactions using an **Electrode Surface Coupling** node in the Transport of Diluted Species interface.

The Electrode Surface boundary of the lithium metal electrode is grounded, whereas an **Electrode Current** boundary condition is used to set the total battery current on the current collector boundary of the NMC electrode.

The battery model is first used in a time-dependent study to perform a 2C discharge simulation from fully charged conditions.

In a second study, an EIS simulation is performed using an **AC Impedance, Initial Values** study at a 50% lithiation level of the NMC electrode.

SOLID MECHANICS MODEL

The local concentration of intercalated lithium in the particles is solved for during the discharge simulation. As the concentration levels in the particles change, the particles will either expand or contract. By coupling the strain of the particles to the local concentration levels, a stress-strain analysis of the binder and particles can be performed.

The **Solid Mechanics** interface is used to perform the stress-strain analysis, using separate **Linear Elastic Material** domain nodes for the separator, porous conductive binder and particle domains.

An **Interpolation** function is used to define the relation between strain and the intercalated lithium concentration of the NMC particles, as shown in Figure 2. This function is then

used to define the strain in the particles using an **Intercalation Strain** subnode to a **Linear Elastic Material**.

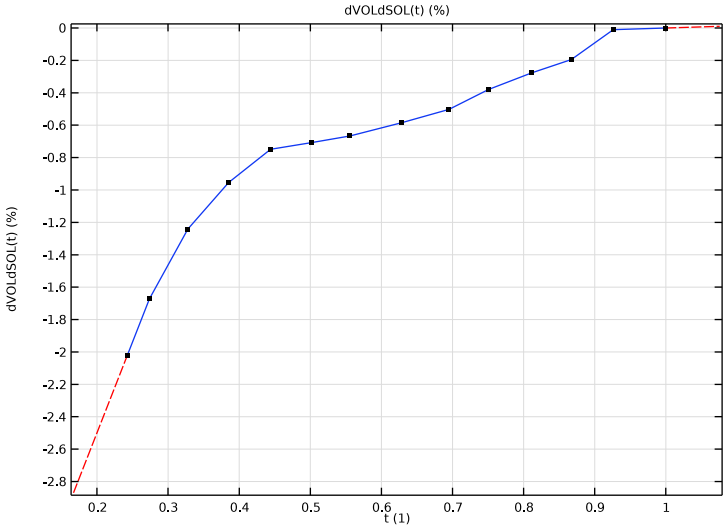


Figure 2: Strain versus intercalation level for NMC. The data was taken from Ref. 3.

Figure 3 shows the cell voltage during the 2C discharge.

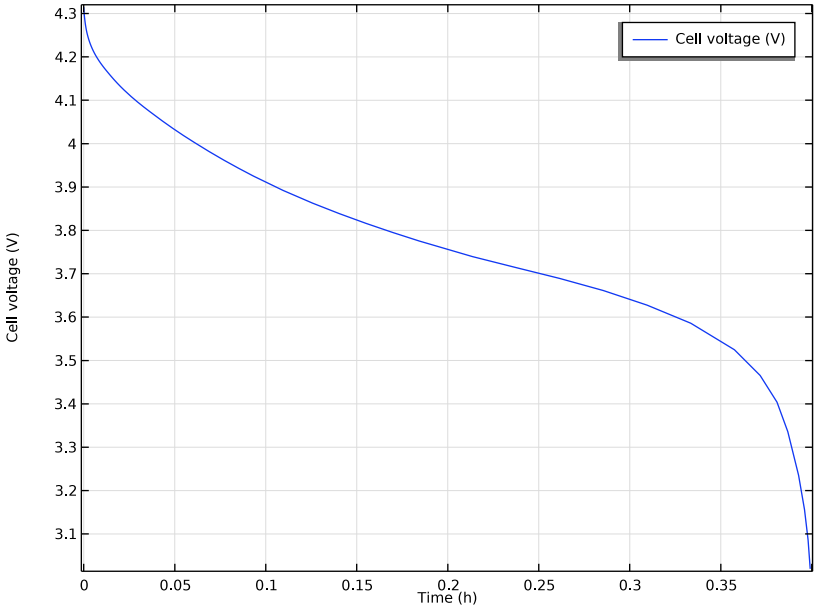


Figure 3: Cell voltage during the 2C discharge.

Figure 4 shows the concentration of intercalated lithium in the particles, as well as the flux and concentration of lithium ions in the electrolyte halfway into the 2C discharge. During discharge, lithium dissolves in an anodic reaction at the lithium metal foil and is subsequently transported as ions toward the NMC particles. At the surface of the NMC materials, cathodic charge transfer occurs, and the formed lithium atoms intercalate and diffuse toward the interior of the particles.

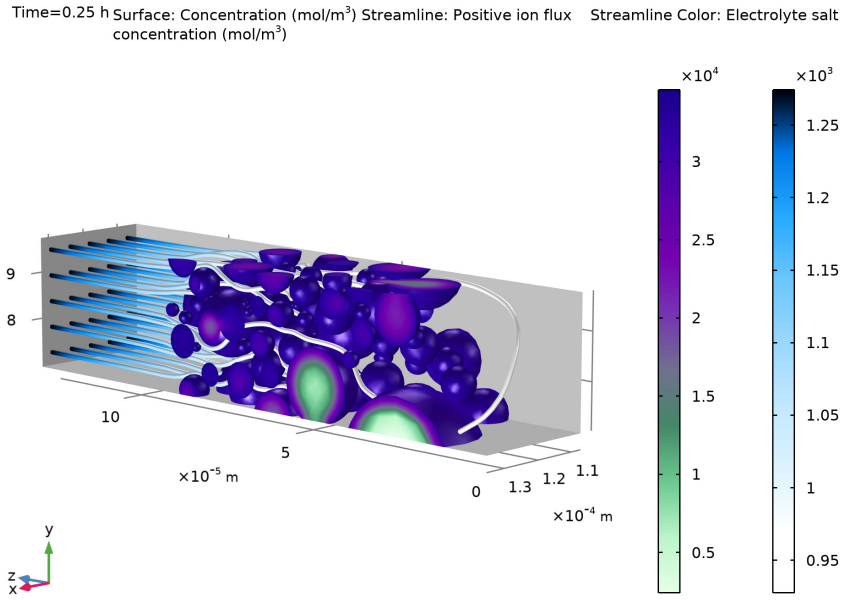


Figure 4: Concentration of intercalated lithium in the particles, and lithium-ion flux streamlines, halfway into the 2C discharge. The color expression of the flux streamlines depict the lithium-ion concentration in the electrolyte.

Figure 5 shows the Nyquist plot from the EIS simulation. The half-circle stems from the charge transfer reaction at the NMC particles, whereas the approx 45° tail is related to the diffusion of intercalated lithium in the particles.

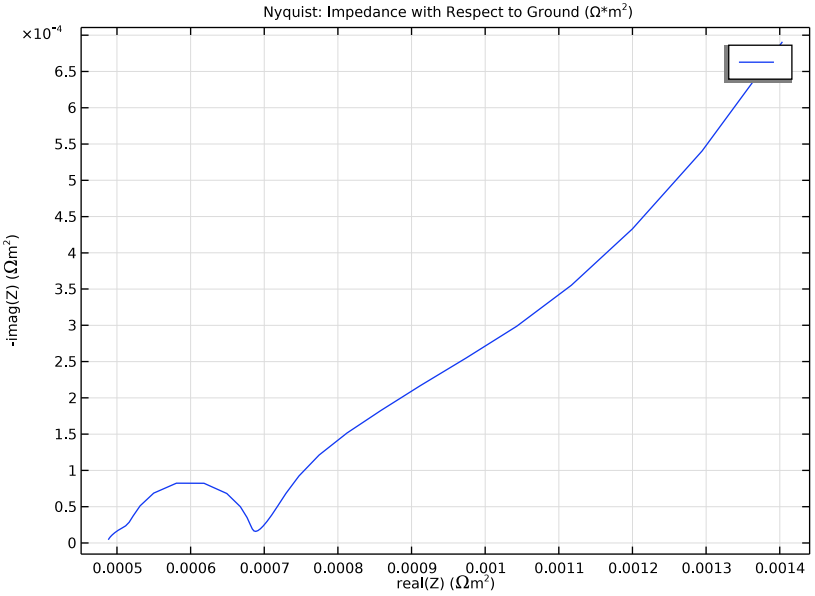


Figure 5: Nyquist plot of the impedance with respect to ground at the NMC current collector.

Figure 6 and Figure 7 show the stresses in the particles and porous conductive binder, respectively, halfway into the 2C discharge.

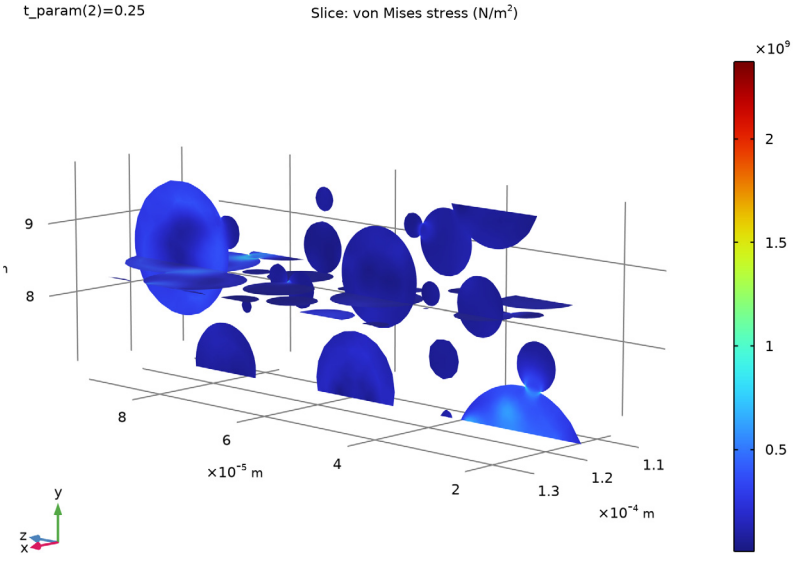


Figure 6: Particle stress halfway into the 2C discharge.

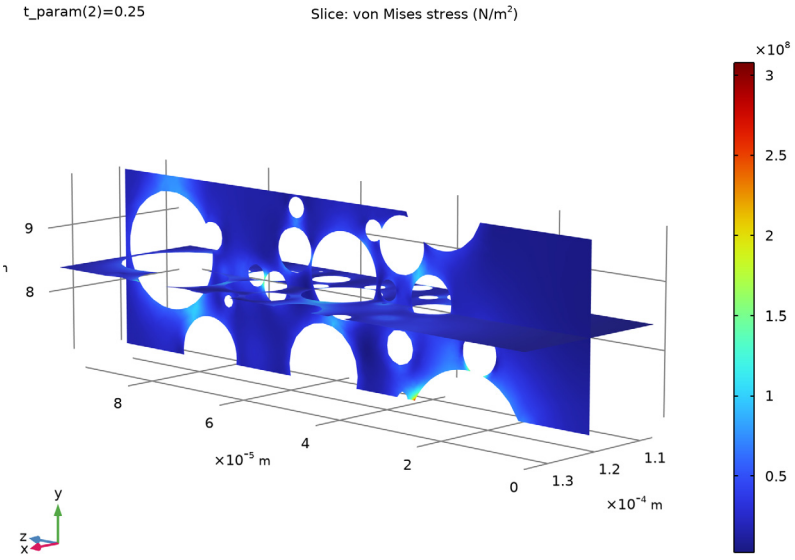


Figure 7: Binder stress halfway into the 2C discharge.

References

1. A. Schmidt, E. Ramani, T. Carraro, J. Joos, A. Weber, M. Kamlah, and E. Ivers-Tiffée, "Understanding Deviations between Spatially Resolved and Homogenized Cathode Models of Lithium-Ion Batteries", *Energy Technol.* 2021, 2000881

2. M.Ebner, F. Geldmacher , F. Marone , M. Stampanoni, and V. Wood, "X-Ray Tomography of Porous, Transition Metal Oxide Based Lithium Ion Battery Electrodes," *Adv. Energy Mater.*, vol. 3, pp. 845–850, 2013. See also supporting information at https://onlinelibrary.wiley.com/doi/abs/10.1002/aenm.201200932

3. R. Koerver and others, "Chemo-mechanical expansion of lithium electrode materials — on the route to mechanically optimized all-solid-state batteries," *Energy Environ. Sci.*, vol. 11, pp. 2142–2158, 2018.

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

ROOT

Start by opening the file containing the heterogeneous electrode geometry.

APPLICATION LIBRARIES

1 From the **File** menu, choose **Application Libraries**.

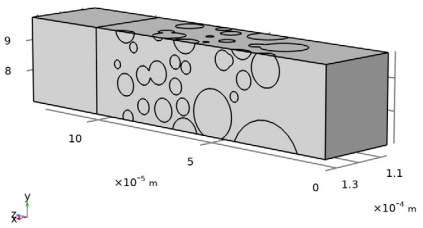
2 In the **Application Libraries** window, select **Battery Design Module>Batteries, Heterogeneous>nmc_electrode_geometry** in the tree.

3 Click **Open**.

GEOMETRY 1

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

2 Right-click **Component 1 (comp1)>Geometry 1** and choose **Build All**.



3 Click the **Wireframe Rendering** button in the **Graphics** toolbar.

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

COMPONENT 1 (COMP1)

For setting up the physics, use the **Lithium-Ion Battery** interface and the **Transport of Diluted Species** interfaces.

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 **Electrochemistry>Batteries>Lithium-Ion Battery (liion)**.

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

5 In the tree, select **Chemical Species Transport>Transport of Diluted Species (tds)**.

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

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

GLOBAL DEFINITIONS

Add the electrode parameters from a text file.

Electrode Parameters

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

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

3 Click **Load from File**.

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

5 In the **Label** text field, type `Electrode Parameters`.

MATERIALS

Add the materials for the electrodes and electrolyte from the material library.

ADD MATERIAL

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

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

3 In the tree, select **Battery>Electrodes>Lithium Metal, Li (Negative, Li-ion Battery)**.

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

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

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

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

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

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

MATERIALS

Lithium Metal, Li (Negative, Li-ion Battery) (mat1)

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

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

3 From the **Selection** list, choose **Lithium Foil**.

NMC 111, LiNi0.33Mn0.33Co0.33O2 (Positive, Li-ion Battery) (mat2)

1 In the **Model Builder** window, click **NMC 111, LiNi0.33Mn0.33Co0.33O2 (Positive, Li-ion Battery) (mat2)**.

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

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

LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery) (mat3)

1 In the **Model Builder** window, click **LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery) (mat3)**.

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

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

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 **Separator + Binder**.

4 Click to expand the **Discretization** section. Reduce the discretization to use linear elements for the battery interface. This will reduce the memory requirements for solving the model. Transport of Diluted species uses linear elements by default and needs not to be altered.

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

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

7 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 **Electrolyte Properties** section.

3 From the **Electrolyte material** list, choose **LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery) (mat3)**.

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 **Electrolyte Properties** section. From the **Electrolyte material** list, choose **LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery) (mat3)**.

5 Locate the **Conductive Binder Properties** section. In the σ_s text field, type `sigma_s`.

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

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

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

Internal Electrode Surface 1

Use the **Internal Electrode Surface** node to model the electrode-electrolyte interface between the particles and the porous conductive binder domain.

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

Set the model input concentration, which is used by the active **Material** to calculate the equilibrium potential, to the concentration variable `c` solved for by the **Transport of Diluted Species** interface.

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 **Material** section. From the **Material** list, choose **NMC 111, LiNi0.33Mn0.33Co0.33O2 (Positive, Li-ion Battery) (mat2)**.

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

6 In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0_ref_NMC`.

Electrode Surface 1

Use an **Electrode Surface** node to model the external lithium foil electrode.

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

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

3 From the **Selection** list, choose **Lithium Foil**.

Electrode Reaction 1

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

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

3 In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0_ref_Li`.

The **Electrode Surface** node is grounded by default. Use an **Electrode Current** node to define the cell current at the positive current collector boundary.

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 **NMC Current Collector**.

4 Locate the **Electrode Current** section. In the $I_{\mathrm{s,total}}$ text field, type `-I_1C*C_rate`.

Set the initial values for the electric potential, both on the boundary and in the domain.

5 In the $\phi_{\mathrm{s,bnd,init}}$ text field, type `mat2.elpot.Eeq_int1(cs0/csmax)`.

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 *phis* text field, type `mat2.elpot.Eeq_int1(cs0/csmax)`.

TRANSPORT OF DILUTED SPECIES (TDS)

Now define the diffusion of intercalated lithium in the particles.

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

2 In the **Settings** window for **Transport of Diluted Species**, locate the **Domain Selection** section.

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

4 Locate the **Transport Mechanisms** section. Clear the **Convection** check box.

Transport Properties 1

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**, locate the **Diffusion** section.

3 From the **Material** list, choose **NMC 111, LiNi0.33Mn0.33Co0.3302 (Positive, Li-ion Battery) (mat2)**.

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

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`.

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**.

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_c text field, type `1`.

DEFINITIONS

Global Variable Probe - E cell

Add a probe for the cell voltage. The probe variable value will be stored in a table for every time step taken by the time-dependent solver.

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

2 In the **Settings** window for **Global Variable Probe**, type `Global Variable Probe - E cell` in the **Label** text field.

3 Locate the **Expression** section. In the **Expression** text field, type `liion.phis0_ec1`.

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

MESH 1

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

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

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

Size

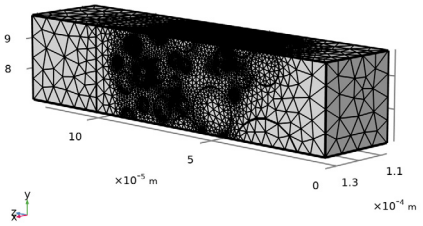
1 In the **Model Builder** window, under **Component 1 (comp1)>Mesh 1** click **Size**.

2 In the **Settings** window for **Size**, click to expand the **Element Size Parameters** section.

3 In the **Maximum element size** text field, type `hmax`.

4 In the **Minimum element size** text field, type `hmin`.

5 Click **Build All**.



ADD STUDY

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

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

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

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

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

STUDY 1 - BATTERY DISCHARGE

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

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

Step 1: Current Distribution Initialization

1 In the **Model Builder** window, under **Study 1 - Battery 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 From the **Time unit** list, choose **h**.

4 In the **Output times** text field, type `0 0.1/C_rate 0.5/C_rate 0.9/C_rate`.

Solution 1 (sol1)

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

Add a stop condition to define a cutoff voltage while discharging.

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

3 Right-click **Study 1 - Battery Discharge>Solver Configurations>Solution 1 (sol1)>Time-Dependent Solver 1** and choose **Stop Condition**.

4 In the **Settings** window for **Stop Condition**, locate the **Stop Expressions** section.

5 Click **Add**.

6 In the table, enter the following settings:

Stop expression	Stop if	Active	Description
`comp1.liion.phis0_ec 1<3[V]`	True (>=1)	√	`Stop expression 1`

7 Locate the **Output at Stop** section. Clear the **Add warning** check box.

Step 2: Time Dependent

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

2 In the **Settings** window for **Time Dependent**, click to expand the **Results While Solving** section.

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

Solution 1 (sol1)

Place the electrolyte concentration dependent variable in a separate segregated group. This will decrease the memory requirements of the solver.

1 In the **Model Builder** window, expand the **Study 1 - Battery Discharge> Solver Configurations>Solution 1 (sol1)>Time-Dependent Solver 1>Segregated 1** node.

2 Right-click **Study 1 - Battery Discharge>Solver Configurations>Solution 1 (sol1)>Time-Dependent Solver 1>Segregated 1** and choose **Segregated Step**.

3 In the **Settings** window for **Segregated Step**, locate the **General** section.

4 In the **Variables** list, select **Electrolyte salt concentration (comp1.cl)**.

5 Under **Variables**, click **Delete**.

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

7 In the **Settings** window for **Segregated Step**, locate the **General** section.

8 Under **Variables**, click **Add**.

9 In the **Add** dialog box, select **Electrolyte salt concentration (comp1.cl)** in the **Variables** list.

10 Click **OK**.

11 In the **Settings** window for **Segregated Step**, locate the **General** section.

12 From the **Linear solver** list, choose **Direct, concentrations (tds)**.

13 In the **Model Builder** window, click **Study 1 - Battery Discharge**.

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

15 Clear the **Generate default plots** check box.

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

RESULTS

The probe plot is automatically generated as shown in (Figure 3).

Discharge voltage

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

2 In the **Settings** window for **1D Plot Group**, type `Discharge voltage` in the **Label** text field.

3 In the **Discharge voltage** toolbar, click **Plot**.

Solid Lithium Concentration and Lithium Ion Flux

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

Start plotting the concentration and the flux for the lithium ion in the heterogeneous electrode. (Figure 4).

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

3 Locate the **Data** section. From the **Time (h)** list, choose **0.25**.

4 Locate the **Plot Settings** section. Clear the **Plot dataset edges** check box.

Surface 1

1 Right-click **Solid Lithium Concentration and Lithium Ion Flux** and choose **Surface**.

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

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

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

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

6 Click **OK**.

Streamline 1

1 In the **Model Builder** window, right-click **Solid Lithium Concentration and Lithium Ion 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 `25`.

4 Locate the **Selection** section. From the **Selection** list, choose **Lithium Foil**.

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

Color Expression 1

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

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

3 In the **Expression** text field, type `c1`.

4 Click to expand the **Title** section. From the **Title type** list, choose **Automatic**.

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

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

7 Click **OK**.

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

9 From the **Color table transformation** list, choose **Reverse**.

Surface 2

1 In the **Model Builder** window, right-click **Solid Lithium Concentration and Lithium Ion Flux** and choose **Surface**.

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

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

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

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

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

Selection 1

1 Right-click **Surface 2** and choose **Selection**.

2 Select Boundaries 1, 2, 16, 17, and 19 only.

3 In the **Solid Lithium Concentration and Lithium Ion Flux** toolbar, click **Plot**.

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

LITHIUM-ION BATTERY (LIION)

Now start setting up the model for the EIS simulation.

Electrode Current 1

Add a harmonic perturbation to perturb the current signal around the stationary value, which is zero current at open circuit in this case.

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

Harmonic Perturbation 1

1 In the **Physics** toolbar, click **Attributes** and choose **Harmonic Perturbation**.

2 In the **Settings** window for **Harmonic Perturbation**, locate the **Harmonic Perturbation** section.

3 In the $\Delta I_{s,total}$ text field, type `I_1C/100`.

Add a double layer capacitance at the NMC surface.

Internal Electrode Surface 1

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

Double-Layer Capacitance 1

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

2 In the **Settings** window for **Double-Layer Capacitance**, locate the **Double-Layer Capacitance** section.

3 In the C_{dl} text field, type `C_dl_NMC`.

4 Locate the **Stoichiometric Coefficient** section. In the ν_{Li+} text field, type `-1`.

GLOBAL DEFINITIONS

Electrode Parameters

Modify the initial state of charge to 50% lithiation before setting up the EIS study.

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

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
socinit	socmin*0+0.5	0.5	Initial lithiation level, nmc (use 0.5 for EIS study, socmin for discharge)

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 **Empty Study**.

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

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

STUDY 2 - EIS

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

Step 1: Frequency-Domain Perturbation

1 In the **Study** toolbar, click **Study Steps** and choose **Frequency Domain>Frequency-Domain Perturbation**.

2 In the **Settings** window for **Frequency-Domain Perturbation**, locate the **Study Settings** section.

3 In the **Frequencies** text field, type `10^range(-2.6,0.2,5)`.

4 Click to expand the **Results While Solving** section. From the **Probes** list, choose **None**.

5 In the **Model Builder** window, collapse the **Study 2 - EIS** node.

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

RESULTS

Impedance with Respect to Ground, Nyquist (liion)

1 In the **Impedance with Respect to Ground, Nyquist (liion)** toolbar, click **Plot**.

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

GLOBAL DEFINITIONS

Solid Mechanics Parameters

Now set up the stress-strain model in the particles using the **Solid Mechanics** interface. Start by importing the parameters for the solid mechanics model.

1. In the **Home** toolbar, click **Parameters** and choose **Add>Parameters**.
2. In the **Settings** window for **Parameters**, type `Solid Mechanics 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 `nmc_electrode_solid_mechanics_parameters.txt`.

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)

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_separator`.
4. From the ν list, choose **User defined**. In the associated text field, type `nu_separator`.
5. From the ρ list, choose **User defined**. In the associated text field, type `rho_separator`.

Linear Elastic Material - Binder

1. In the **Physics** toolbar, click **Domains** and choose **Linear Elastic Material**.
2. In the **Settings** window for **Linear Elastic Material**, type `Linear Elastic Material - Binder` in the **Label** text field.
3. Locate the **Domain Selection** section. From the **Selection** list, choose **Porous Conductive Binder**.

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

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

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

Linear Elastic Material 3

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

The strain in the particles depends on the concentration of intercalated lithium. First inspect the volumetric strain vs the lithiation level function, defined in the NMC material.

MATERIALS

NMC 111, LiNi0.33Mn0.33Co0.33O2 (Positive, Li-ion Battery) (mat2)

In the **Model Builder** window, expand the **NMC 111, LiNi0.33Mn0.33Co0.33O2 (Positive, Li-ion Battery) (mat2)** node.

Interpolation 1 (dVOLdSOL)

1 In the **Model Builder** window, expand the **Component 1 (comp1)>Materials>NMC 111, LiNi0.33Mn0.33Co0.33O2 (Positive, Li-ion Battery) (mat2)> Intercalation strain (IntercalationStrain)** node, then click **Interpolation 1 (dVOLdSOL)**.

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

The function plot is shown in Figure 2.

SOLID MECHANICS (SOLID)

Linear Elastic Material - Particles

1 In the **Model Builder** window, under **Component 1 (comp1)>Solid Mechanics (solid)** click **Linear Elastic Material 3**.

2 In the **Settings** window for **Linear Elastic Material**, type `Linear Elastic Material - Particles` in the **Label** text field.

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

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

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 **All External Boundaries**.

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 3 - SOLID MECHANICS

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

2 In the **Settings** window for **Study**, type `Study 3 - Solid Mechanics` in the **Label** text field.

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

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
t_param (Time parameter for Solid Mechanics analysis (in hours))	`0.1/C_rate 0.5/C_rate 0.9/C_rate`	

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

Stationary - Solid Mechanics

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

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

3 Locate the **Physics and Variables Selection** section. 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 - Battery Discharge, Time Dependent**.

7 From the **Time (h)** list, choose **Interpolated**.

8 In the **Time** text field, type `t_param`.

Solution 4 (sol4)

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

2 In the **Model Builder** window, expand the **Solution 4 (sol4)** node.

By enabling the iterative solver, the memory requirements are reduced.

3 In the **Model Builder** window, expand the **Study 3 - Solid Mechanics> Solver Configurations>Solution 4 (sol4)>Stationary Solver 1** node.

4 Right-click **Study 3 - Solid Mechanics>Solver Configurations>Solution 4 (sol4)> Stationary Solver 1>Suggested Iterative Solver (solid)** and choose **Enable**.

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

RESULTS

Stress, Particles

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

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

3 Locate the **Data** section. From the **Dataset** list, choose **Study 3 - Solid Mechanics/ Parametric Solutions 1 (sol5)**.

4 From the **Parameter value (t_param)** list, choose **0.25**.

5 Locate the **Plot Settings** section. Clear the **Plot dataset edges** check box.

Slice 1

1 Right-click **Stress, Particles** and choose **Slice**.

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

3 In the **Expression** text field, type `solid.mises`.

4 Locate the **Plane Data** section. From the **Plane** list, choose **ZX-planes**.

5 In the **Planes** text field, type `1`.

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 **Particles**.

4 In the **Stress, Particles** toolbar, click **Plot**.

Slice 1

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

Slice 2

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

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

3 From the **Plane** list, choose **YZ-planes**.

4 In the **Planes** text field, type `1`.

5 Click to expand the **Inherit Style** section. From the **Plot** list, choose **Slice 1**.

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

7 In the **Stress, Particles** toolbar, click **Plot**.

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

This plot visualizes the stress in the particles. (Figure 6).

Stress, Particles

In the **Model Builder** window, right-click **Stress, Particles** and choose **Duplicate**.

Stress, Binder

1 In the **Model Builder** window, under **Results** click **Stress, Particles 1**.

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

Slice 1

In the **Model Builder** window, expand the **Stress, Binder** node.

Selection 1

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

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

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

Selection 1

1 In the **Model Builder** window, expand the **Results>Stress, Binder>Slice 2** node, then click **Selection 1**.

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

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

4 In the **Stress, Binder** toolbar, click **Plot**.

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

This plots visualizes the stress in the binder domain. (Figure 7).