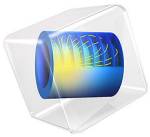


Homogenizing a Heterogeneous Electrode Model

Introduction

This example demonstrates how to calculate the effective transport properties of a heterogeneous 3D geometry of an nickel manganese cobalt (NMC) electrode. The effective flux parameter is then used to create a representative homogenized 1D model of the NMC electrode.

By homogenizing, memory requirements and computational times are reduced by orders of magnitude.

See also the *Heterogeneous NMC Electrode* tutorial for how to define the corresponding heterogeneous model.

Model Definition

Figure 1 shows the 3D geometry generated from tomography data (Ref. 1) 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.

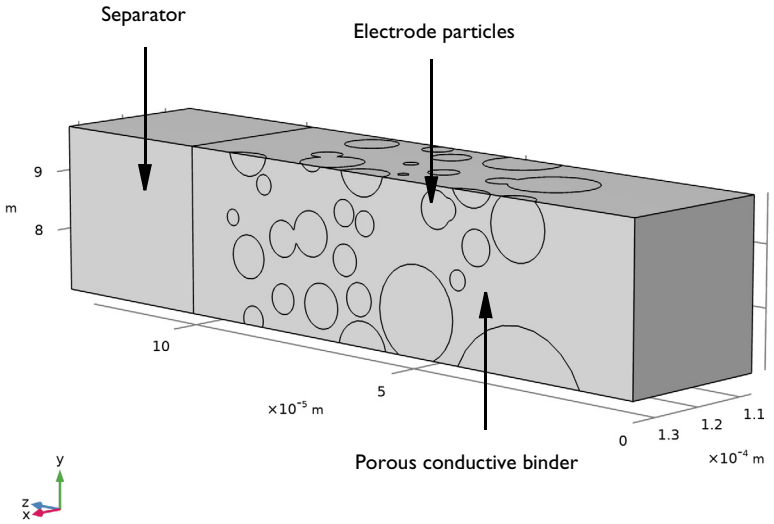


Figure 1: Model geometry.

MODEL FOR CALCULATING EFFECTIVE TRANSPORT PARAMETERS

The homogenized model of the NMC electrode uses one single domain to define all transport processes occurring in the electrode and electrolyte phases. The homogenized equations make use of effective (volume-averaged) transport parameters, which are calculated by multiplying the diffusivity and conductivities of the porous conductive binder by an effective flux parameter f_{eff}. This parameter is also sometimes referred to as the McMullin number (Ref. 2).

The effective flux parameter will depend on both the volume fraction, ε , and the tortuosity, τ, of the porous conductive binder domain according to

$$f_{\text{eff}} = \frac{\varepsilon}{\tau} \tag{1}$$

For a homogeneous domain (that is, with no particles present) with volume fraction and tortuosity both equal to unity, $f_{\text{eff}} = 1$.

To calculate the effective transport coefficient for the porous conductive domain, we will solve for Laplace's equation (that is, a diffusion equation with the diffusion coefficient equal to unity) using the dependent variable u.

$$-\nabla \cdot \nabla u = 0 \tag{2}$$

in the porous conductive binder domain together with the boundary conditions

$$u = 0 \tag{3}$$

at the boundary facing the separator and

$$u = 1 \tag{4}$$

at the boundary facing the NMC current collector.

By integrating the flux in the solved model at the NMC current collector boundary, our effective flux parameter f_{elec} can be calculated as

$$f_{\text{eff}} = L_{\text{elec}} \int_A -\nabla u \cdot \mathbf{n} dA \tag{5}$$

HOMOGENIZED BATTERY MODEL

Figure 2 shows the 1D homogenized model geometry.

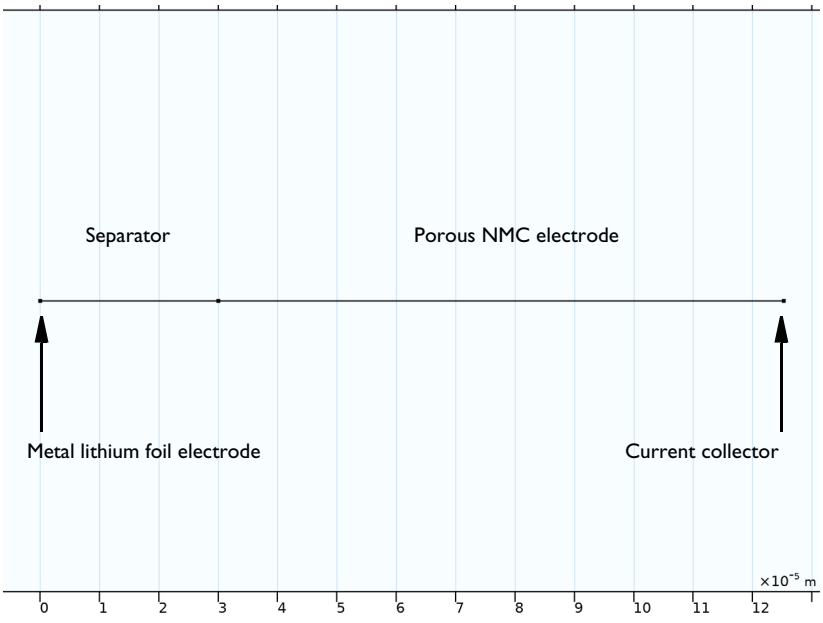


Figure 2: 1D geometry used in the homogenized model.

The model is defined using the **Lithium-Ion Battery** interface similarly to the *Heterogeneous NMC Electrode* tutorial, with the following differences:

- The **Porous Electrode** node is used to define the homogenized mixture of electrode particles, binder and electrolyte material of the electrode, considering the volume fractions of the electrode and electrolyte phases in the 3D geometry and the effective flux parameter f_{eff} .
- A **Porous Electrode Reaction** child node to the **Porous Electrode** defines the equilibrium potential, and the electrode kinetics using a specific surface area parameter based on the 3D geometry.
- The diffusion of solid lithium is solved for using an extra dimension defined by the **Particle Intercalation** child node to the **Porous Electrode**, using an average particle radius that was calculated by the model method when creating the 3D geometry. (In the *Heterogeneous NMC Electrode* tutorial a separate **Transport of Diluted Species** interface was used to model the intercalated lithium diffusion.)

For more details on this homogenized 1D approach to lithium battery cell modeling, see the *1D Isothermal Lithium-Ion Battery* tutorial.

Similarly to the heterogeneous tutorial, two simulations are run: A 2C discharge from 100% state-of-charge (SOC), and an electrochemical impedance spectroscopy (EIS) simulation at 50% SOC.

Results and Discussion

Figure 3 shows the Laplacian flux through the porous conductive binder domain. Integrating the flux on the boundary and using Equation 5 results in the value f_{eff}=0.55.

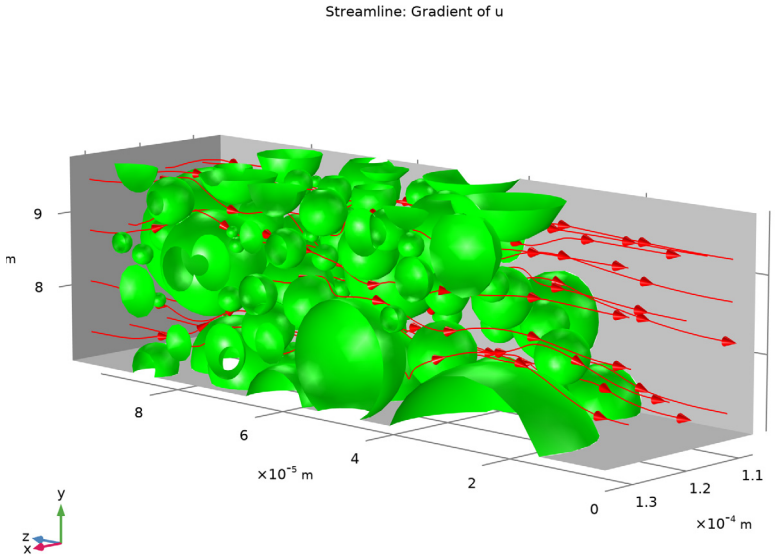


Figure 3: Flux through the porous conductive binder domain when solving for Laplace's equation.

Figure 4 shows the 2C discharge curve of the battery, and compares the result to the heterogeneous model. The resulting discharge voltages of the two models match well during the discharge, apart from the final part of the discharge, where diffusion limitations of intercalated lithium in the largest particles of the heterogeneous model result in a faster drop of the discharge voltage. (Increasing the average radius parameter of the homogeneous model about 20% will make the two curves more or less overlap in this case.)

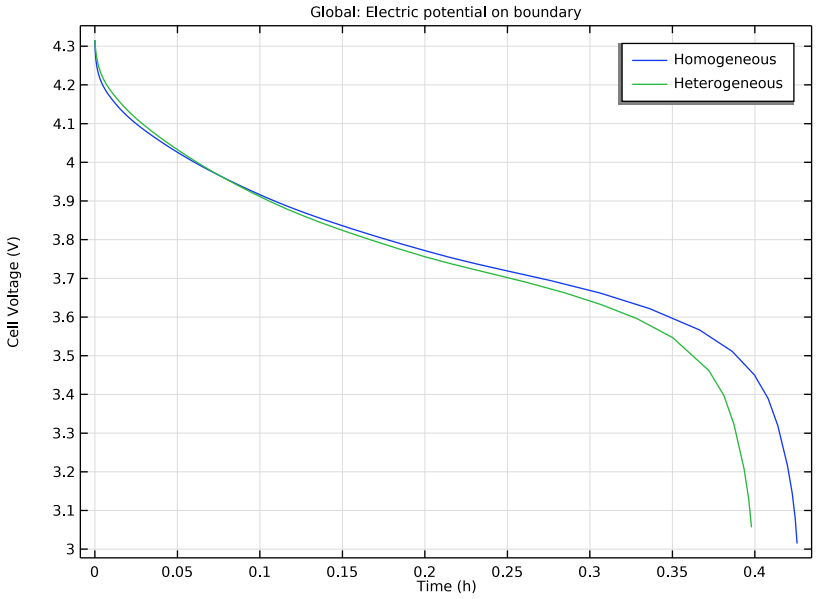


Figure 4: 2C discharge curves comparing the results from the homogenized model to the original heterogeneous model.

Figure 5 shows the Nyquist plot from the EIS simulation, compared to the heterogeneous model results. The two semicircles, related to the charge transfer, more or less overlap,

whereas the approx 45° tail, related to the intercalated lithium diffusion, show larger differences between the two models.

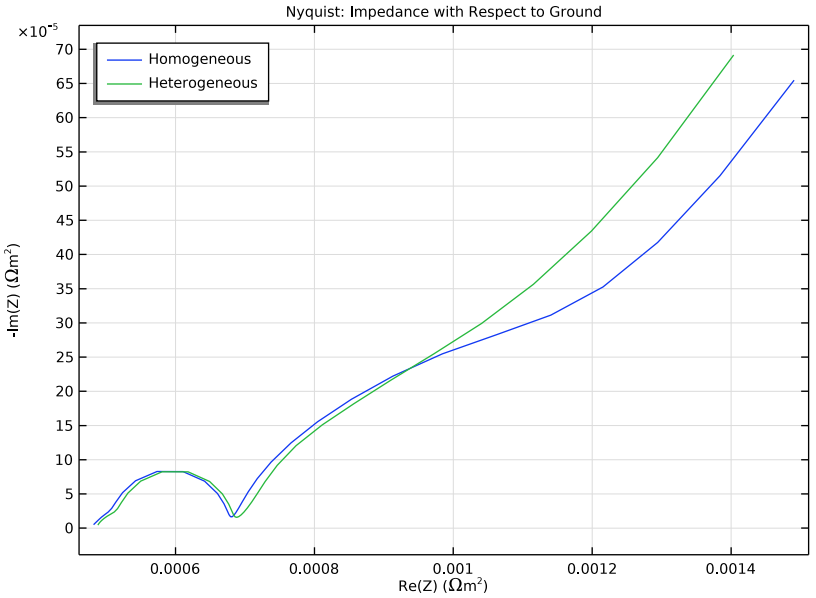


Figure 5: Nyquist plot from the EIS simulations at 50% lithiation of the NMC particles, comparing the results of the homogeneous model to the original heterogeneous model.

Reference

1. 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

2. 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

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

APPLICATION LIBRARIES

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

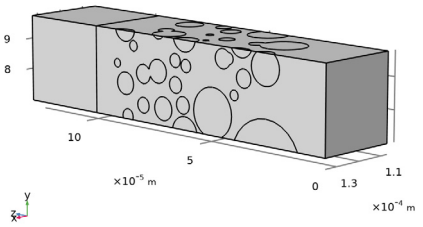
2 In the **Application Libraries** window, select **Battery Design Module>Batteries, Heterogeneous>nmc_electrode_geometry** in the tree.

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.

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 **Mathematics>Classical PDEs>Laplace's Equation (lpeq)**.

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

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

LAPLACE'S EQUATION (LPEQ)

1 In the **Settings** window for **Laplace's Equation**, locate the **Domain Selection** section.

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

Dirichlet Boundary Condition 1

1 Right-click **Component 1 (comp1)>Laplace's Equation (lpeq)** and choose **Dirichlet Boundary Condition**.

2 Select Boundary 18 only.

Dirichlet Boundary Condition 2

1 In the **Physics** toolbar, click **Boundaries** and choose **Dirichlet Boundary Condition**.

2 Select Boundary 3 only.

3 In the **Settings** window for **Dirichlet Boundary Condition**, locate the **Dirichlet Boundary Condition** section.

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

MESH 1

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

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

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

Size

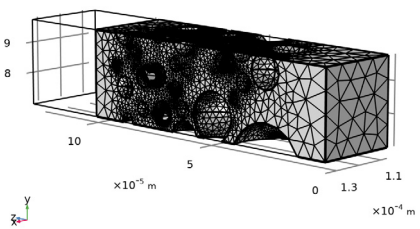
1 In the **Model Builder** window, under **Component 1 (comp1)>Mesh 1** click **Size**.

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 **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 1

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

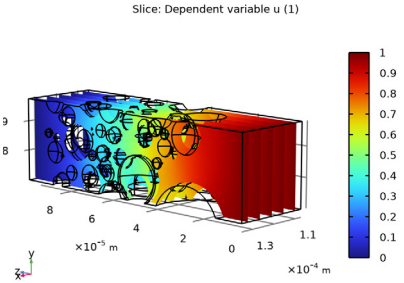
RESULTS

Dependent Variable u

Inspect the default plot for the dependent variable u.

1 In the **Settings** window for **3D Plot Group**, type `Dependent Variable u` in the **Label** text field.

2 In the **Dependent Variable u** toolbar, click **Plot**.



Flux

Create a streamline plot of the flux (Figure 3) as follows:

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

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

Streamline 1

1 Right-click **Flux** and choose **Streamline**.

2 Select Boundary 18 only.

3 In the **Settings** window for **Streamline**, locate the **Coloring and Style** section.

4 Find the **Point style** subsection. From the **Type** list, choose **Arrow**.

5 In the **Flux** toolbar, click **Plot**.

Surface 1

1 In the **Model Builder** window, right-click **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 **Green**.

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

Selection 1

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

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

3 From the **Selection** list, choose **Particle Surfaces**.

4 In the **Flux** toolbar, click **Plot**.

Surface 2

1 In the **Model Builder** window, right-click **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**.

6 Locate the **Title** section. From the **Title type** list, choose **None**.

Selection 1

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

2 Select Boundaries 1, 2, and 18 only.

3 In the **Flux** toolbar, click **Plot**.

Flux

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

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

3 Clear the **Plot dataset edges** check box.

4 In the **Flux** toolbar, click **Plot**.

Surface Average - Effective Flux Factor

Calculate the effective flux factor through the porous conductive binder as follows:

1 In the **Results** toolbar, click **More Derived Values** and choose **Average> Surface Average**.

2 In the **Settings** window for **Surface Average**, type `Surface Average - Effective Flux Factor` in the **Label** text field.

3 Select Boundary 3 only.

4 Click **Replace Expression** in the upper-right corner of the **Expressions** section. From the menu, choose **Component 1 (comp1)>Laplace's Equation>dflux.u - Boundary flux down direction - 1/m**.

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

Expression	Unit	Description
dflux.u*L_elec	1	Effective flux factor

6 Click **Evaluate**.

Make a note of the derived value in **Table 2**, and add the corresponding `f_eff` parameter to use in the homogenized model as follows:

GLOBAL DEFINITIONS

Geometry Parameters

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

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
f_eff	0.554	0.554	Effective flux factor

Electrode Parameters

Import some additional parameters for the homogenized model.

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

2 In the **Settings** window for **Parameters**, type `Electrode 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_parameters.txt`.

ROOT

The homogenized 1D model is placed in a separate component.

ADD COMPONENT

In the **Model Builder** window, right-click the root node and choose **Add Component>1D**.

GEOMETRY 2

Interval 1 (i1)

1 In the **Model Builder** window, under **Component 2 (comp2)** right-click **Geometry 2** and choose **Interval**.

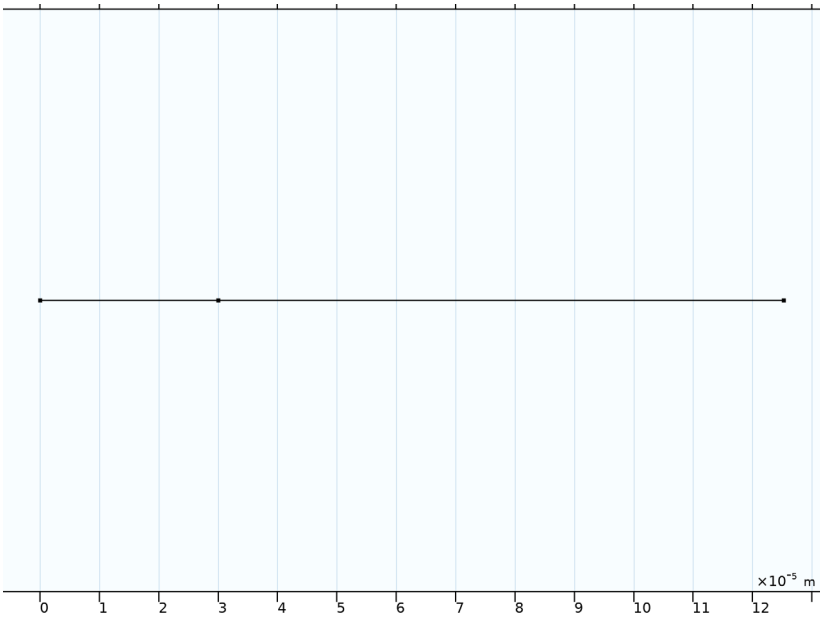
2 In the **Settings** window for **Interval**, locate the **Interval** section.

3 From the **Specify** list, choose **Interval lengths**.

4 In the table, enter the following settings:

Lengths (m)
L_sep
L_elec

5 Click **Build Selected**.



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 2** in the window toolbar.

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

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

4 Right-click and choose **Add to Component 2 (comp2)**.

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

6 Right-click and choose **Add to Component 2 (comp2)**.

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 2 (comp2)**.

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

MATERIALS

Lithium Metal, Li (Negative, Li-ion Battery) (mat2)

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

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

3 Select Boundary 1 only.

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 **All domains**.

LITHIUM-ION BATTERY (LIION)

1 In the **Model Builder** window, under **Component 2 (comp2)** click **Lithium-Ion Battery (liion)**.

2 In the **Settings** window for **Lithium-Ion Battery**, locate the **Cross-Sectional Area** section.

3 In the A_c text field, type `A_cross`.

Separator 1

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

2 Select Domain 1 only.

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

4 In the ε_l text field, type `epsl_sep`.

Porous Electrode 1

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

2 Select Domain 2 only.

3 In the **Settings** window for **Porous Electrode**, locate the **Electrode Properties** section.

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

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

6 In the ε_l text field, type `eps_l_b*eps_binder`.

7 Locate the **Effective Transport Parameter Correction** section. From the **Electrolyte conductivity** list, choose **User defined**. In the f_l text field, type `f_eff*(eps_l_b^1.5)`.

8 From the **Electrical conductivity** list, choose **User defined**. In the f_s text field, type `f_eff`.

9 From the **Diffusion** list, choose **User defined**. In the f_{Dl} text field, type `f_eff*(eps_l_b^1.5)`.

Particle Intercalation 1

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

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

3 From the **Particle material** list, choose **NMC 111, LiNi0.33Mn0.33Co0.33O2 (Positive, Li-ion Battery) (mat1)**.

4 Locate the **Species Settings** section. In the $c_{s,init}$ text field, type `cs0`.

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

Porous Electrode Reaction 1

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

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

3 From the **Material** list, choose **NMC 111, LiNi0.33Mn0.33Co0.33O2 (Positive, Li-ion Battery) (mat1)**.

4 Locate the **Electrode Kinetics** section. In the $i_{0,ref}(T)$ text field, type `i0_ref_NMC`.

5 Locate the **Active Specific Surface Area** section. From the **Active specific surface area** list, choose **User defined**. In the a_v text field, type `Av_particles`.

Electrode Surface 1

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

2 Select Boundary 1 only.

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`.

Electrode Current 1

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

2 Select Boundary 3 only.

3 In the **Settings** window for **Electrode Current**, locate the **Electrode Current** section.

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

DEFINITIONS (COMP2)

Integration 1 (intop1)

1 In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **Integration**.

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

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

4 Select Boundary 3 only.

5 In the **Operator name** text field, type `intop_nmc_cc`.

ADD STUDY

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

Solve the homogenized model in a new study. Disable the Laplace equation in this study.

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

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

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

5 In the **Model Builder** window, click the root node.

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

STUDY 2

Step 1: Current Distribution Initialization

1 In the **Settings** window for **Current Distribution Initialization**, locate the **Physics and Variables Selection** section.

2 In the table, clear the **Solve for** check box for **Laplace's Equation (lpeq)**.

3 Click to expand the **Mesh Selection** section. Disabling the mesh in Geometry 1, which is not used by the homogenized model, memory can be saved.

4 In the table, enter the following settings:

Component	Mesh
Component 1	No mesh

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 `range(0,0.1/C_rate,0.9/C_rate)`.

5 Locate the **Physics and Variables Selection** section. In the table, clear the **Solve for** check box for **Laplace's Equation (lpeq)**.

6 Click to expand the **Mesh Selection** section. In the table, enter the following settings:

Component	Mesh
Component 1	No mesh

Solution 2 (sol2)

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

2 In the **Model Builder** window, expand the **Solution 2 (sol2)** node, then click **Time-Dependent Solver 1**.

3 In the **Settings** window for **Time-Dependent Solver**, locate the **General** section.

4 From the **Times to store** list, choose **Steps taken by solver**.

5 Right-click **Study 2>Solver Configurations>Solution 2 (sol2)>Time-Dependent Solver 1** and choose **Stop Condition**.

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

7 Click **Add**.

8 In the table, enter the following settings:

Stop expression	Stop if	Active	Description
`comp2.intop_nmc_cc(comp2.phis)<3[V]`	True (>=1)	√	`Stop expression 1`

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

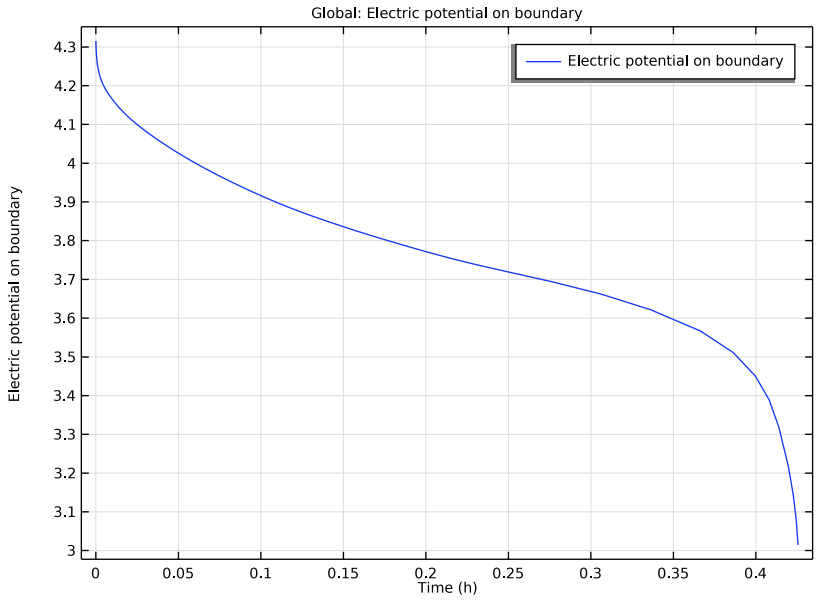
10 In the **Study** toolbar, click **Compute**.

RESULTS

Boundary Electrode Potential with Respect to Ground (liion)

The discharge voltage is plotted by default.

1 In the **Boundary Electrode Potential with Respect to Ground (liion)** toolbar, click **Plot**.



LITHIUM-ION BATTERY (LIION)

Now start setting up the EIS simulation.

Porous Electrode 1

In the **Model Builder** window, under **Component 2 (comp2)>Lithium-Ion Battery (liion)** click **Porous Electrode 1**.

Porous Matrix Double Layer Capacitance 1

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

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

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

4 From the **Double layer area** list, choose **User defined**. In the $a_{\mathrm{v,dl}}$ text field, type `Av_particles`.

Electrode Current - Harmonic Perturbation

1 In the **Model Builder** window, under **Component 2 (comp2)>Lithium-Ion Battery (liion)** right-click **Electrode Current 1** and choose **Duplicate**.

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

3 Locate the **Electrode Current** section. In the $I_{\mathrm{s,total}}$ text field, type `0`.

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 $\Delta I_{\mathrm{s,total}}$ text field, type `I_1C/20`.

GLOBAL DEFINITIONS

Electrode Parameters

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 **Preset Studies for Some Physics Interfaces>AC Impedance, Initial Values**.

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

5 In the **Model Builder** window, click the root node.

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

STUDY 3

Step 1: Frequency Domain Perturbation

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

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

3 Locate the **Physics and Variables Selection** section. In the table, clear the **Solve for** check box for **Laplace's Equation (lpeq)**.

4 Click to expand the **Mesh Selection** section. In the table, enter the following settings:

Component	Mesh
Component 1	No mesh

Current Distribution Initialization

1 In the **Study** toolbar, click **Study Steps** and choose **Other> Current Distribution Initialization**.

2 Right-click **Study 3>Step 2: Current Distribution Initialization** and choose **Move Up**.

3 In the **Settings** window for **Current Distribution Initialization**, locate the **Physics and Variables Selection** section.

4 In the table, clear the **Solve for** check box for **Laplace's Equation (lpeq)**.

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

Component	Mesh
Component 1	No mesh

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

RESULTS

Heterogeneous Discharge Data (Imported)

1 In the **Results** toolbar, click **Table**.

2 In the **Settings** window for **Table**, type `Heterogeneous Discharge Data (Imported)` in the **Label** text field.

3 Locate the **Data** section. Click **Import**.

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

Heterogeneous EIS Data (Imported)

1 In the **Results** toolbar, click **Table**.

2 In the **Settings** window for **Table**, type `Heterogeneous EIS Data (Imported)` in the **Label** text field.

3 Locate the **Data** section. Click **Import**.

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

Discharge Voltage

1 In the **Model Builder** window, under **Results** click **Boundary Electrode Potential with Respect to Ground (liion)**.

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

3 Locate the **Plot Settings** section.

4 Select the **y-axis label** check box. In the associated text field, type `Cell Voltage (V)`.

Table Graph 1

1 Right-click **Discharge Voltage** and choose **Table Graph**.

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

3 From the **Table** list, choose **Heterogeneous Discharge Data (Imported)**.

4 Click to expand the **Legends** section. Select the **Show legends** check box.

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

6 In the table, enter the following settings:

Legends
Heterogeneous

Global 1

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

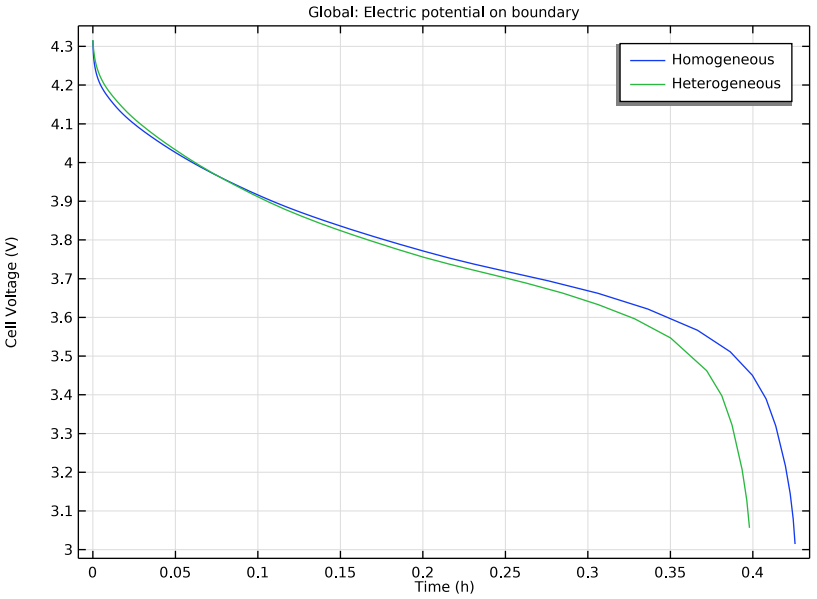
2 In the **Settings** window for **Global**, click to expand the **Legends** section.

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

4 In the table, enter the following settings:

Legends
Homogeneous

5 In the **Discharge Voltage** toolbar, click **Plot**.



Impedance with Respect to Ground, Nyquist (liion)

We can compare the Nyquist plots from both the heterogeneous and the homogeneous approach (Figure 5).

1 In the **Model Builder** window, expand the **Results>Impedance with Respect to Ground, Nyquist (liion)** node, then click **Impedance with Respect to Ground, Nyquist (liion)**.

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

3 Select the **x-axis label** check box. In the associated text field, type `Re(Z) (\Omega m<sup>2</sup>)`.

4 Select the **y-axis label** check box. In the associated text field, type `-Im(Z) (\Omega m<sup>2</sup>)`.

5 Locate the **Legend** section. From the **Position** list, choose **Upper left**.

Table Graph 1

1 Right-click **Impedance with Respect to Ground, Nyquist (liion)** and choose **Table Graph**.

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

3 From the **Table** list, choose **Heterogeneous EIS Data (Imported)**.

4 From the **x-axis data** list, choose **Imaginary Part of Z (Ω*m^2)** **Real Part of Z (Ω*m^2)**.

5 From the **Plot columns** list, choose **Manual**.

6 In the **Columns** list, select **Column 2**.

7 Locate the **Legends** section. Select the **Show legends** check box.

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

9 In the table, enter the following settings:

Legends
Heterogeneous

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

Nyquist 1

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

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

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

4 In the table, enter the following settings:

Legends
Homogeneous

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