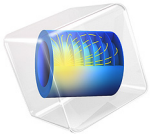


Internal Short Circuit in a Lithium-Ion Battery

Introduction

During an internal short circuit of a battery the two electrode materials are internally interconnected electronically, giving rise to high local current densities. Internal short circuits may occur in a lithium-ion battery due to, for instance, lithium dendrite formation or a compressive shock. A prolonged internal short circuit results in self discharge in combination with a local temperature increase. The latter phenomena is of great importance since the electrolyte may start to decompose by exothermic reactions if the temperature reaches above a certain threshold level, causing thermal runaway with potential health and safety hazards.

This model example investigates the local temperature rise due to the occurrence of a penetrating metallic filament in the separator between the two porous electrode materials.

Model Definition

The model geometry is modeled as a layered disk made in 2D with axial symmetry. The penetrating filament is placed at r=0 and has the same height as the separator domain. The

disk, with a cross-sectional area of about 1.3 mm^2, is assumed to be a part of a much larger battery with a cross-sectional area in the order of 0.1 m^2, or higher.

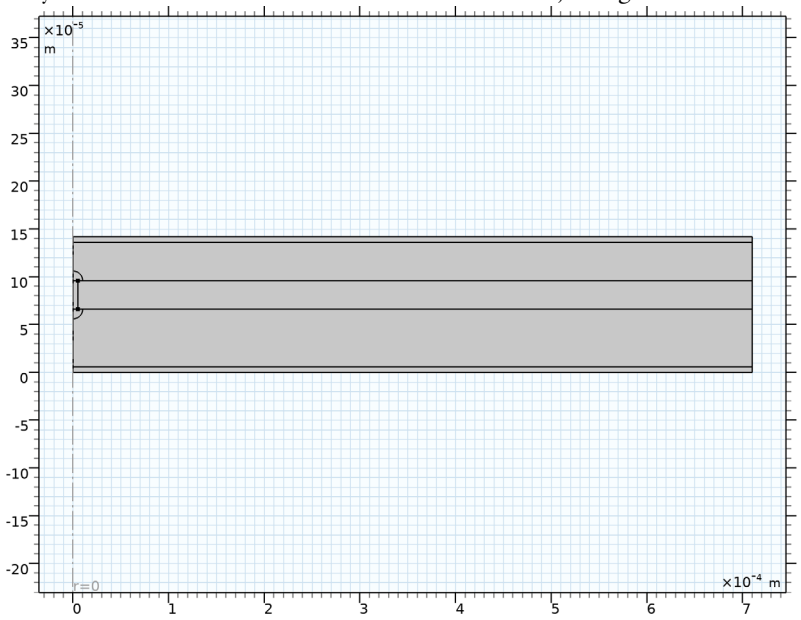


Figure 1: Model geometry. The rectangular layers represent (from the bottom): negative current collector, negative porous electrode, separator, positive porous electrode, positive current collector. The penetrating filament is placed at r=0 and has the same height as the separator domain.

The physics is set up by a Lithium-Ion Battery interface coupled to a Heat Transfer interface. The battery chemistry consists of a graphite negative electrode (50 µm thick) and a NMC positive electrode (40 µm thick) with LiPF6 electrolyte in 3:7 EC:EMC solvent (separator thickness 30 µm). 6 µm thick aluminum and copper current collectors are used on the positive and negative sides, respectively.

The total short-circuit current (< 10 mA) is assumed to be relatively low in relation to the total capacity (> 1 Ah) of the battery, so that over the investigated time period (0.1 s), the battery voltage outside the disk can be assumed to be constant. A constant cell potential is hence set on the outer radius of the disk. It is also assumed that the total heat capacity of the parts of the battery outside the modeled disk geometry, in combination with the high thermal conductivity of the metal foils, will result in the temperature of the outer rim of the disk to be constant during the simulated time period. Some of the temperature material parameters are taken from Ref. 1

The conductivity of the penetrating filament is set to a very low value at t=0 and ramped up to full conductivity at t=0.001 s using a smoothed step function.

Two different radii of the penetrating filament are investigated: 0.1 and 5 µm.

Results and Discussion

Figure 2 shows the temperature distribution at t=0.1 s for a penetrating filament radius of 5 µm. The maximum temperature is located close to the penetrating filament. The temperature change is confined to a small space close to the filament.

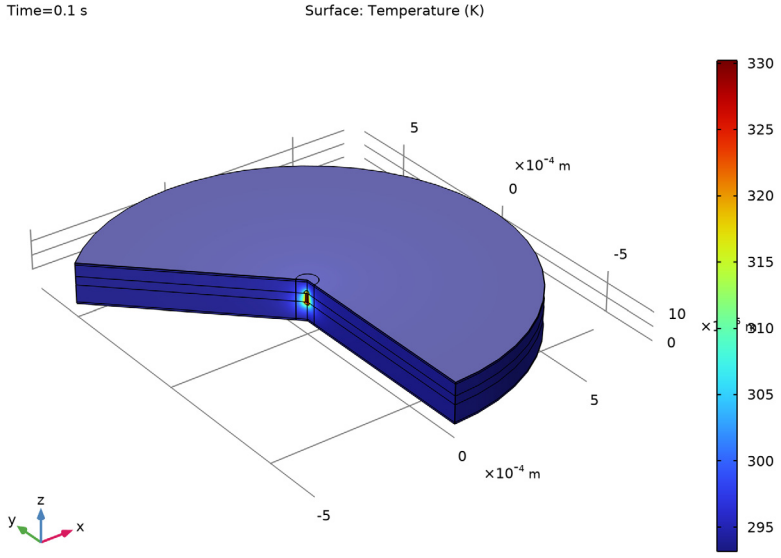


Figure 2: Temperature after 0.1 s for a radius of 5 µm.

Figure 3 shows the temperature distribution along the separator-positive electrode boundary.

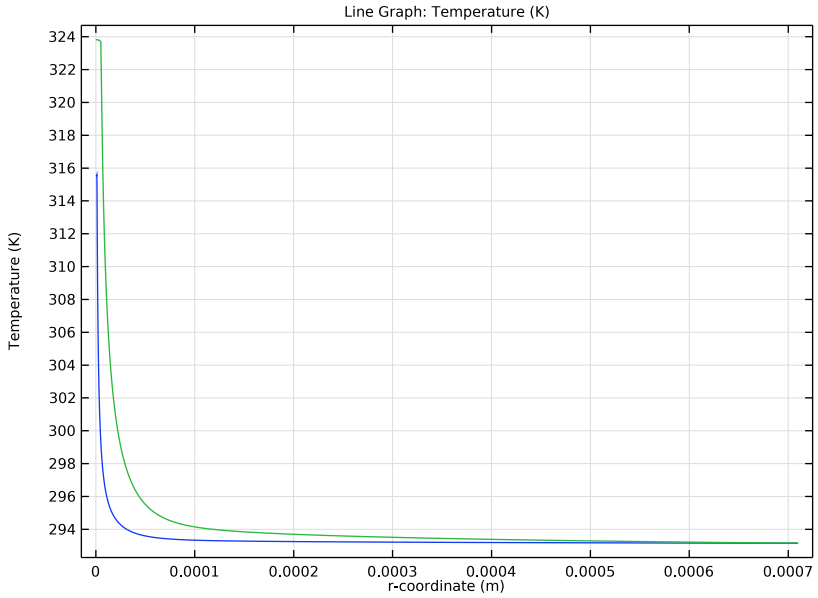


Figure 3: Temperature along the separator-positive electrode boundary.

Figure 4 shows the local state-of-charge for a penetrating filament radius of 5 µm at t=0.1 s. Outside the close vicinity to the penetrating filament the battery is uniformly discharged. A conclusion from this (which would also be confirmed by analyzing the total current flowing through the nail in relation to the integrated reaction currents in the electrodes) is that it would suffice to use a secondary current distribution (that is, ignoring local concentration changes) to analyze the thermal behavior due to the short circuit. The

dominating heat source is the ohmic heating in the filament and electrode phase close to the filament.

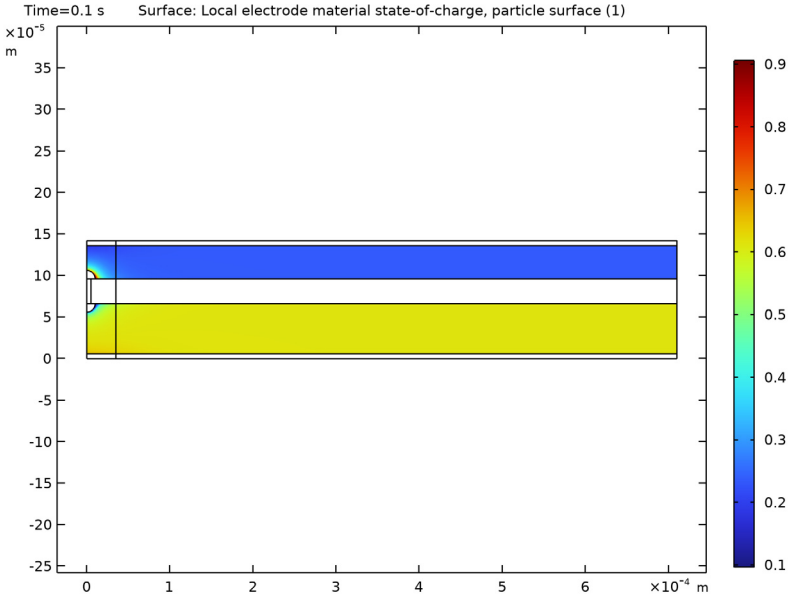


Figure 4: Local state of charge at t=0.1 s for a radius of 5 μm.

Figure 5 compares the maximum temperature in the cell for the two radii of the penetrating filament. The thicker radius causes a higher maximum temperature. This is related to the higher cross sectional area, resulting in a higher total short-circuit current.

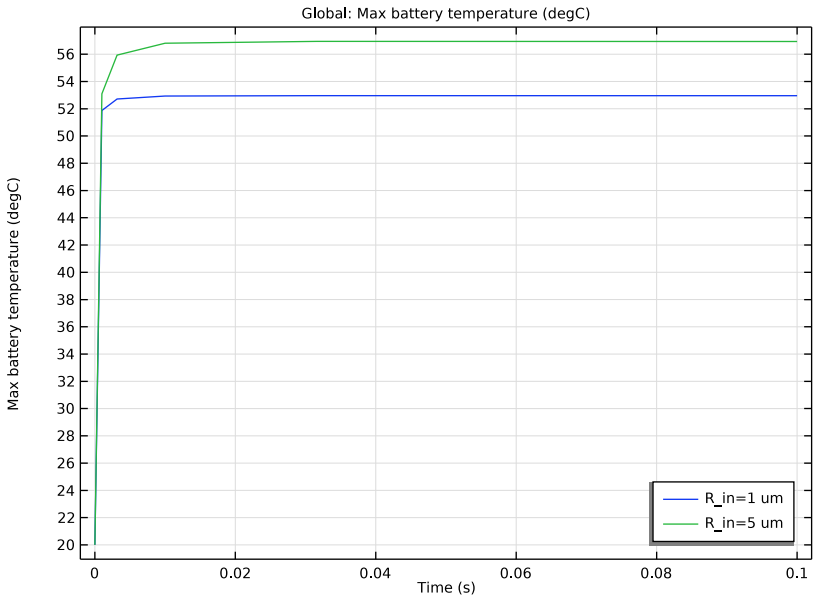


Figure 5: Maximum cell temperature versus time.

Notes About the COMSOL Implementation

The parts of the porous electrodes closest to the shorting filaments are made inactive in the model. This is to facilitate numerical convergence.

Reference

1. *Investigation of Short-Circuit Scenarios in a Lithium-Ion Battery Cell,* T. Zavalis, M. Behm, and G. Lindbergh, *Journal of the Electrochemical Society*, vol. 159, no. 6, pp A848–A859, 2012.

Application Library path: `Battery_Design_Module/Batteries,_Lithium-Ion/internal_short_circuit`

From the **File** menu, choose **New**.

NEW

In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, click **2D Axisymmetric**.

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

3 Click **Add**.

4 In the **Select Physics** tree, select **Heat Transfer>Heat Transfer in Solids (ht)**.

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**.

ROOT

Load the model parameters from a text file.

GLOBAL DEFINITIONS

Parameters 1

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

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

3 Click **Load from File**.

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

GEOMETRY 1

Rectangle 1 (r1)

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

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

3 In the **Width** text field, type `R_out`.

4 In the **Height** text field, type `L_tot`.

5 Click to expand the **Layers** section. In the table, enter the following settings:

Layer name	Thickness (m)
Layer 1	L_negCC
Layer 2	L_neg
Layer 3	L_sep
Layer 4	L_pos

6 Click **Build Selected**.

Polygon 1 (pol1)

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

2 In the **Settings** window for **Polygon**, locate the **Object Type** section.

3 From the **Type** list, choose **Open curve**.

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

r (m)	z (m)
R_in	L_negCC+L_neg
R_in	L_negCC+L_neg+L_sep

Circle 1 (c1)

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

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

3 In the **Radius** text field, type R_in*2.

4 In the **Sector angle** text field, type 90.

5 Locate the **Position** section. In the **z** text field, type L_negCC+L_neg+L_sep.

Circle 2 (c2)

1 Right-click **Circle 1 (c1)** and choose **Duplicate**.

2 In the **Settings** window for **Circle**, locate the **Position** section.

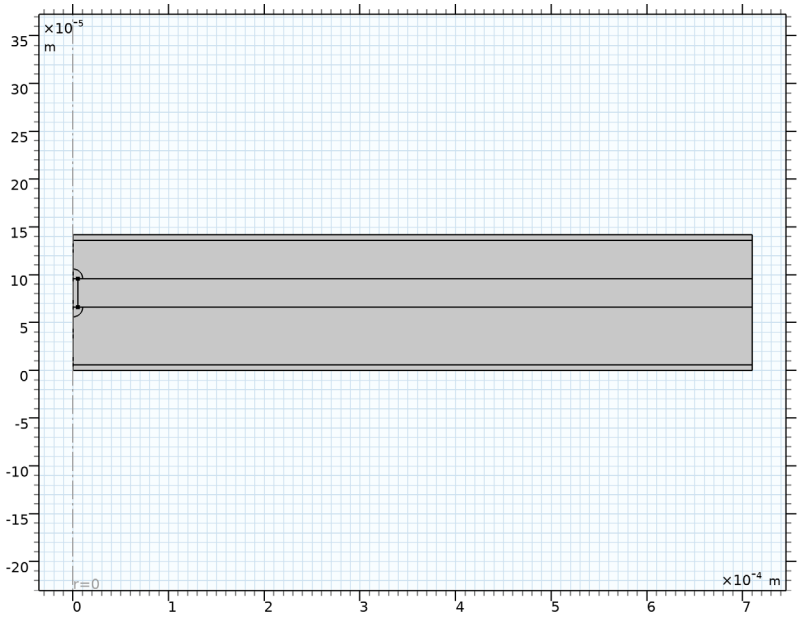
3 In the **z** text field, type L_negCC+L_neg.

4 Locate the **Rotation Angle** section. In the **Rotation** text field, type 270.

5 Click **Build Selected**.

6 Click **Build Selected**.

The geometry should now look like this:



Polygon 2 (pol2)

Finally also add a vertical line that will be used when meshing.

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

2 In the **Settings** window for **Polygon**, locate the **Object Type** section.

3 From the **Type** list, choose **Open curve**.

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

r (m)	z (m)
R_in+L_sep	0
R_in+L_sep	L_tot

5 Click **Build Selected**.

DEFINITIONS

Now create a number of selections on the geometry. These will be used later on when setting up the physics.

Negative CC

1 In the **Definitions** toolbar, click **Explicit**.

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

3 Select Domains 1 and 9 only.

Negative Electrode

1 In the **Definitions** toolbar, click **Explicit**.

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

3 Select Domains 2, 3, and 10 only.

Separator

1 In the **Definitions** toolbar, click **Explicit**.

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

3 Select Domains 8 and 11 only.

Positive Electrode

1 In the **Definitions** toolbar, click **Explicit**.

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

3 Select Domains 5, 6, and 12 only.

Positive CC

1 In the **Definitions** toolbar, click **Explicit**.

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

3 Select Domains 7 and 13 only.

Penetrating Filament

1 In the **Definitions** toolbar, click **Explicit**.

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

3 Select Domain 4 only.

Metal Conductor Domains

1 In the **Definitions** toolbar, click **Union**.

2 In the **Settings** window for **Union**, type `Metal Conductor Domains` in the **Label** text field.

3 Locate the **Input Entities** section. Under **Selections to add**, click **Add**.

4 In the **Add** dialog box, in the **Selections to add** list, choose **Negative CC**, **Positive CC**, and **Penetrating Filament**.

5 Click **OK**.

Negative Terminal

1 In the **Definitions** toolbar, click **Explicit**.

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

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

4 Select Boundary 30 only.

Positive Terminal

1 In the **Definitions** toolbar, click **Explicit**.

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

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

4 Select Boundary 34 only.

Terminals

1 In the **Definitions** toolbar, click **Union**.

2 In the **Settings** window for **Union**, type `Terminals` in the **Label** text field.

3 Locate the **Geometric Entity Level** section. From the **Level** list, choose **Boundary**.

4 Locate the **Input Entities** section. Under **Selections to add**, click **Add**.

5 In the **Add** dialog box, in the **Selections to add** list, choose **Negative Terminal** and **Positive Terminal**.

6 Click **OK**.

MATERIALS

Now add some materials 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 **Built-in>Aluminum**.

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

5 In the tree, select **Built-in>Copper**.

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

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

8 Click **Add to Component** in the window toolbar.

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

10 Click **Add to Component** in the window toolbar.

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

12 Click **Add to Component** in the window toolbar.

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

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

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

MATERIALS

Now assign the added materials to different parts of the geometry.

Aluminum (mat1)

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

2 From the **Selection** list, choose **Positive CC**.

Copper (mat2)

1 In the **Model Builder** window, click **Copper (mat2)**.

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

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

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 **Positive Electrode**.

Graphite, LixC6 MCMB (Negative, Li-ion Battery) (mat4)

1 In the **Model Builder** window, click **Graphite, LixC6 MCMB (Negative, Li-ion Battery) (mat4)**.

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

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

LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery) (mat5)

1 In the **Model Builder** window, click **LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery) (mat5)**.

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

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

Lithium Metal, Li (Negative, Li-ion Battery) (mat6)

1 In the **Model Builder** window, click **Lithium Metal, Li (Negative, Li-ion Battery) (mat6)**.

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

3 From the **Selection** list, choose **Penetrating Filament**.

Some of the added materials are marked with a red cross, indicating missing material properties. You will go back at a later stage to fill in the missing values.

LITHIUM-ION BATTERY (LIION)

Now start setting up the physics, beginning with the lithium-ion battery.

Porous Electrode 1 (Negative)

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

2 In the **Settings** window for **Porous Electrode**, type `Porous Electrode 1 (Negative)` in the **Label** text field.

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

4 Locate the **Electrolyte Properties** section. From the **Electrolyte material** list, choose **LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery) (mat5)**.

5 Locate the **Electrode Properties** section. From the **Electrode material** list, choose **Graphite, LixC6 MCMB (Negative, Li-ion Battery) (mat4)**.

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

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

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 **Graphite, LixC6 MCMB (Negative, Li-ion Battery) (mat4)**.

4 Locate the **Particle Transport Properties** section. In the r_p text field, type `rp_neg`.

5 Click to expand the **Heat of Mixing** section. Select the **Include heat of mixing** check box.

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 **Graphite, LixC6 MCMB (Negative, Li-ion Battery) (mat4)**.

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

Porous Electrode 1 (Negative)

Duplicate the node to create the positive porous electrode, and change only the parameters that differ from the negative.

Porous Electrode 2 (Positive)

1. In the **Model Builder** window, right-click **Porous Electrode 1 (Negative)** and choose **Duplicate**.
2. In the **Settings** window for **Porous Electrode**, type `Porous Electrode 2 (Positive)` in the **Label** text field.
3. Locate the **Domain Selection** section. From the **Selection** list, choose **Positive Electrode**.
4. Locate the **Electrode Properties** section. From the **Electrode material** list, choose **NMC 111, LiNi0.33Mn0.33Co0.33O2 (Positive, Li-ion Battery) (mat3)**.
5. Locate the **Porous Matrix Properties** section. In the ε_s text field, type `epss_pos`.
6. In the ε_l text field, type `epsl_pos`.

Particle Intercalation 1

1. In the **Model Builder** window, expand the **Porous Electrode 2 (Positive)** node, then 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) (mat3)**.
4. Locate the **Particle Transport Properties** section. In the r_p text field, type `rp_pos`.

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) (mat3)**.
4. Locate the **Electrode Kinetics** section. In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0ref_pos`.

Porous Electrode 1 (Negative, Electrochemically Inactive)

1. In the **Model Builder** window, right-click **Porous Electrode 1 (Negative)** and choose **Duplicate**.
2. In the **Settings** window for **Porous Electrode**, type `Porous Electrode 1 (Negative, Electrochemically Inactive)` in the **Label** text field.
3. Select Domain 3 only.
4. Locate the **Particle Properties** section. From the list, choose **Nonintercalating particles**.

Porous Electrode Reaction 1

1 In the **Model Builder** window, expand the **Porous Electrode 1 (Negative, Electrochemically Inactive)** node, then click **Porous Electrode Reaction 1**.

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

3 From the E_{eq} list, choose **User defined**. In the associated text field, type `0.1[V]`.

4 Locate the **Electrode Kinetics** section. From the $i_{loc,expr}$ list, choose **User defined**. Click to expand the **Heat of Reaction** section. From the list, choose **User defined**.

Porous Electrode 2 (Positive, Electrochemically Inactive)

1 In the **Model Builder** window, right-click **Porous Electrode 2 (Positive)** and choose **Duplicate**.

2 In the **Settings** window for **Porous Electrode**, type `Porous Electrode 2 (Positive, Electrochemically Inactive)` in the **Label** text field.

3 Select Domain 5 only.

4 Locate the **Particle Properties** section. From the list, choose **Nonintercalating particles**.

Porous Electrode Reaction 1

1 In the **Model Builder** window, expand the **Porous Electrode 2 (Positive, Electrochemically Inactive)** node, then click **Porous Electrode Reaction 1**.

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

3 From the E_{eq} list, choose **User defined**. In the associated text field, type `0.1[V]+ E_cell`.

4 Locate the **Electrode Kinetics** section. From the $i_{loc,expr}$ list, choose **User defined**. Locate the **Heat of Reaction** section. From the list, choose **User defined**.

Electrode 1 (CCs and Filament)

The electronically conducting domains are specified using one common Electrode node. Different material parameters will be specified for these domains in the Materials node.

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

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

3 From the **Selection** list, choose **Metal Conductor Domains**.

4 In the **Label** text field, type `Electrode 1 (CCs and Filament)`.

Separator 1

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

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

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

4 Locate the **Porous Matrix Properties** section. In the ε_l text field, type `epsl_sep`.

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 Terminal**.

Electric Potential 1

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

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

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

4 Locate the **Electric Potential** section. In the $\phi_{s,bnd}$ text field, type `E_cell`.

Use an Initial Cell Charge Distribution node to specify the initial cell voltage and the capacity of the battery.

Initial Cell Charge Distribution 1

1 In the **Physics** toolbar, click **Global** and choose **Initial Cell Charge Distribution**.

2 In the **Settings** window for **Initial Cell Charge Distribution**, locate the **Battery Cell Parameters** section.

3 In the $E_{cell,0}$ text field, type `E_cell`.

4 In the $Q_{cell,0}$ text field, type `Q_batt`.

Negative Electrode Selection 1

1 In the **Model Builder** window, expand the **Initial Cell Charge Distribution 1** node, then click **Negative Electrode Selection 1**.

2 Select Domains 2 and 10 only.

Positive Electrode Selection 1

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

2 Select Domains 6 and 12 only.

HEAT TRANSFER IN SOLIDS (HT)

Now set up the Heat Transfer part of the problem. All domain specific material parameters will be set up by the Materials node, so the default Heat Transfer in Solids node can be used in all domains.

In the **Model Builder** window, under **Component 1 (comp1)** click **Heat Transfer in Solids (ht)**.

Temperature 1

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

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

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

4 Locate the **Temperature** section. In the T_0 text field, type `T0`.

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 T text field, type `T0`.

MULTIPHYSICS

Electrochemical Heating 1 (ech1)

In the **Physics** toolbar, click **Multiphysics Couplings** and choose **Domain> Electrochemical Heating**.

MATERIALS

Now go back to the Materials node and fill in the missing parameters to remove the red crosses.

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

1 In the **Model Builder** window, under **Component 1 (comp1)>Materials** 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	`rho_pos`	kg/m³	Basic
Heat capacity at constant pressure	Cp	`Cp_pos`	J/(kg·K)	Basic

LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery) (mat5)

1 In the **Model Builder** window, click **LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery) (mat5)**.

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
Thermal conductivity	k_iso ; kii = k_iso, kij = 0	k_sep	W/(m·K)	Basic
Density	rho	rho_sep	kg/m³	Basic
Heat capacity at constant pressure	Cp	Cp_sep	J/(kg·K)	Basic

DEFINITIONS (COMP1)

For the electric conductivity of the penetrating filament we will use a step function to ramp up the conductivity at $t = 0$.

Step 1 (step1)

1 In the **Home** toolbar, click f(x) **Functions** and choose **Global>Step**.

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

3 In the **Location** text field, type `0.5`.

4 Click to expand the **Smoothing** section. In the **Size of transition zone** text field, type `1`.

MATERIALS

Lithium Metal, Li (Negative, Li-ion Battery) (mat6)

1 In the **Model Builder** window, under **Component 1 (comp1)>Materials** click **Lithium Metal, Li (Negative, Li-ion Battery) (mat6)**.

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
Electrical conductivity	sigma_iso ; sigmaii = sigma_iso, sigmaij = 0	max(step1(t/t_ramp), 1e-8)/(92.8[nΩ*m])	S/m	Basic

The red cross on the Materials node should now be gone.

MESH 1

Create the mesh using a triangular mesh close to the filament, and then a mapped mesh with a growing element size in the x direction for the remaining domains.

Free Triangular 1

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

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

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

4 Select Domains 1–6 only.

Distribution 1

1 Right-click **Free Triangular 1** and choose **Distribution**.

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

3 Click  **Paste Selection**.

4 In the **Paste Selection** dialog box, type `35 36` in the **Selection** text field.

5 Click **OK**.

6 In the **Settings** window for **Distribution**, locate the **Distribution** section.

7 In the **Number of elements** text field, type `10`.

Mapped 1

1 In the **Mesh** toolbar, click  **Mapped**.

2 In the **Settings** window for **Mapped**, click to expand the **Control Entities** section.

3 Clear the **Smooth across removed control entities** check box.

Distribution 1

1 Right-click **Mapped 1** and choose **Distribution**.

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

3 Click  **Paste Selection**.

4 In the **Paste Selection** dialog box, type `20, 22, 24, 26, 28-29` in the **Selection** text field.

5 Click **OK**.

6 In the **Settings** window for **Distribution**, locate the **Distribution** section.

7 From the **Distribution type** list, choose **Predefined**.

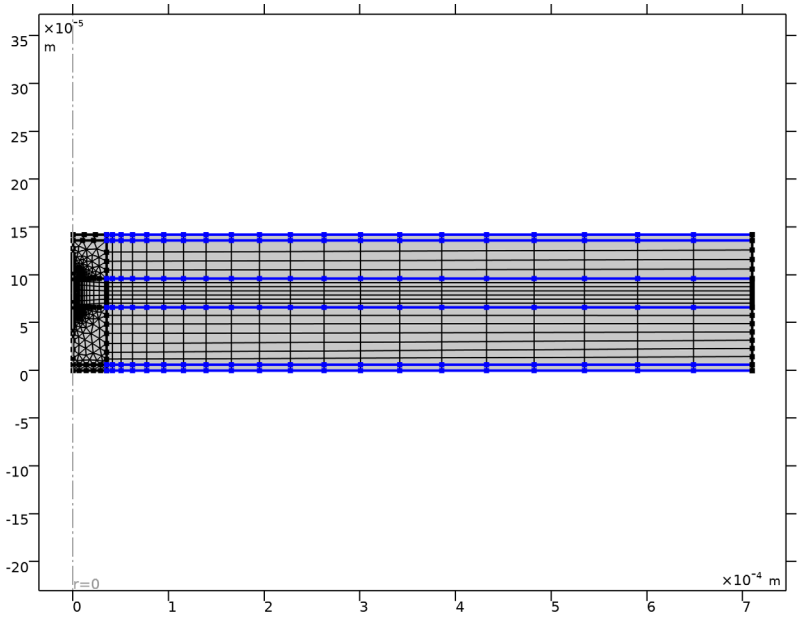
8 In the **Number of elements** text field, type `20`.

9 In the **Element ratio** text field, type `10`.

10 Select the **Reverse direction** check box.

11 Click **Build All**.

The finalized mesh should look like this:



DEFINITIONS (COMP1)

Add a probe to monitor the maximum temperature of the cell while solving.

Max temperature probe

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

2 In the **Settings** window for **Domain Probe**, type `Max temperature probe` in the **Label** text field.

3 Locate the **Probe Type** section. From the **Type** list, choose **Maximum**.

4 Locate the **Expression** section. In the **Expression** text field, type `T`.

Maximum 1 (maxop1)

Also add a maximum operator that will be used while postprocessing once the model is solved.

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

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

3 From the **Selection** list, choose **All domains**.

STUDY 1

The physics and mesh settings are now complete. The model is to be solved in two steps. The first step is used to initialize the battery cell. Turn off solving for Heat Transfer in the first solver step.

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 In the **Output times** text field, type `0 10^range(-3,0.5,-1)`.

Parametric Sweep

Use a Parametric Sweep to solve for two different radii of the penetrating filament.

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
R_in (Inner radius of penetrating filament)	1 5	um

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

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

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

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

RESULTS

Revolution 2D 1

Plot a revolution plot of the temperature (Figure 2) as follows:

1 In the **Results** toolbar, click **More Datasets** and choose **Revolution 2D**.

2 In the **Settings** window for **Revolution 2D**, click to expand the **Revolution Layers** section.

3 In the **Start angle** text field, type `-90`.

4 In the **Revolution angle** text field, type `225`.

Temperature (revolution plot)

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

2 In the **Settings** window for **3D Plot Group**, type `Temperature (revolution plot)` in the **Label** text field.

Surface 1

1 Right-click **Temperature (revolution plot)** and choose **Surface**.

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

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

4 In the **Temperature (revolution plot)** toolbar, click **Plot**.

Temperature along separator

Plot the temperature along the separator-positive electrode boundary (Figure 3) as follows:

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

2 In the **Settings** window for **1D Plot Group**, type `Temperature along separator` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/ Parametric Solutions 1 (sol3)**.

4 From the **Time selection** list, choose **Last**.

Line Graph 1

1 Right-click **Temperature along separator** and choose **Line Graph**.

2 Select Boundaries 9, 16, 18, and 26 only.

3 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

4 In the **Expression** text field, type `T`.

5 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

6 In the **Expression** text field, type `r`.

7 In the **Temperature along separator** toolbar, click **Plot**.

Local soc

Plot the local state-of-charge (Figure 4) as follows:

1 In the **Home** toolbar, click **Add Plot Group** and choose **2D Plot Group**.

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

Surface 1

1 Right-click **Local soc** and choose **Surface**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)>Lithium-Ion Battery>Particle intercalation>liion.socloc_surface - Local electrode material state-of-charge, particle surface**.

3 In the **Local soc** toolbar, click **Plot**.

Max temperature vs. time

Plot the maximum temperature versus time (Figure 5) as follows:

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

2 In the **Settings** window for **1D Plot Group**, type `Max temperature vs. time` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/ Parametric Solutions 1 (sol3)**.

4 Locate the **Legend** section. From the **Position** list, choose **Lower right**.

Global 1

1 Right-click **Max temperature vs. time** and choose **Global**.

2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.

3 In the table, enter the following settings:

Expression	Unit	Description
`comp1.maxop1(T)`	`degC`	`Max battery temperature`

4 Click to expand the **Legends** section. Find the **Include** subsection. Clear the **Description** check box.

5 In the **Max temperature vs. time** toolbar, click **Plot**.