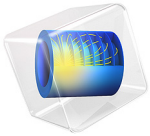


2D Lithium-Ion Battery

Introduction

This tutorial is a two-dimensional model of a lithium-ion battery. The cell geometry could be a small part of an experimental cell, but here it is only meant to demonstrate a 2D model setup. The battery contains a positive porous electrode, electrolyte, a negative lithium metal electrode, and a current collector. This cell configuration is sometimes called a "half-cell", since the lithium metal electrode has negligible impact on cell voltage and polarization. A more realistic 2D geometry is exemplified in the model Edge Effects in a Spirally Wound Lithium-Ion Battery available in the Battery Design Module Application Library.

For a detailed description of this model, in particular step-by-step instructions with several screen shots showing how to build it, see the book *Introduction to the Battery Design Module*.

Model Definition

The 3D cell geometry is shown in Figure 1. Due to symmetry along the height of the battery, the 3D geometry can be modeled using a 2D cross section. Figure 1 shows the positioning of the positive and negative electrodes, and the current collector attached to the positive electrode. The positive electrode is porous and the negative electrode consists of lithium metal. The modeled 2D cross section is highlighted in the light blue section in the rightmost figure of Figure 1.

Since the electrochemical reaction only takes place at the surface of the lithium metal, and the electronic conductivity is very high, the thickness of the metal is neglected in the model geometry. The modeled 2D cell geometry is shown in Figure 2. During discharge, the positive electrode acts as the cathode and the contact of the metallic tab acts as a current collector. The negative lithium metal electrode acts as the anode and current feeder.

The model defines and solves the current and material balances in the lithium-ion battery. The intercalation of lithium inside the particles in the positive electrode is solved using a fourth independent variable for the particle radius (x, y, and t are the other three). The reaction kinetics and the intercalation are coupled to the material and current balances at the surface of the particles. The model equations are found in the *Battery Design Module*

User's Guide. The model equations were originally formulated for 1D simulations by John Newman and his coworkers at the University of California at Berkeley.

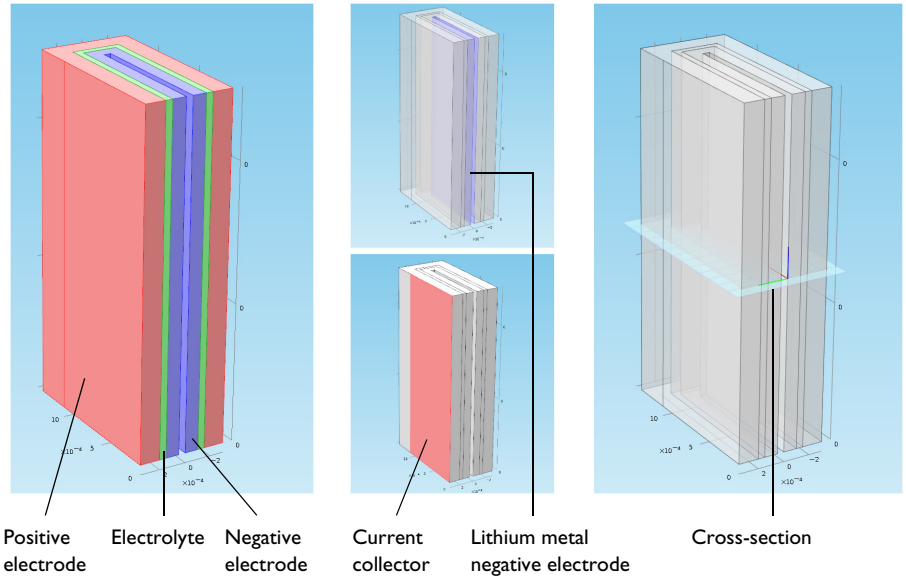


Figure 1: 3D model geometry of Lithium-ion model.

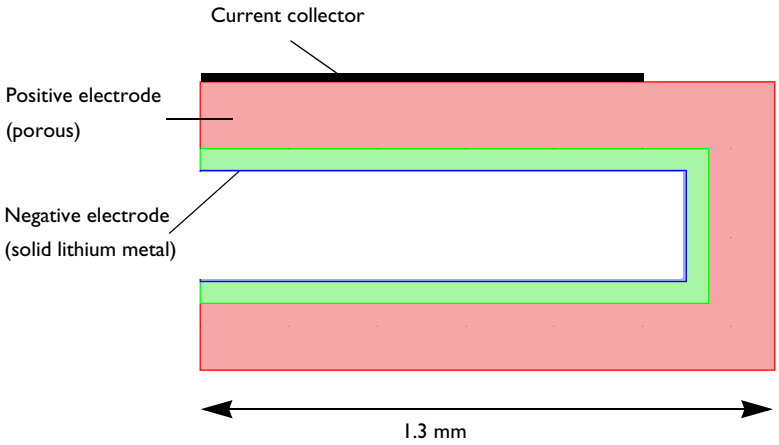


Figure 2: A 2D cross-sectional model geometry with the thickness of the negative lithium metal electrode neglected.

The purpose of the 2D simulation is to reveal the distribution of the depth of discharge in the positive electrode, as a function of discharge time. This distribution depends on the positioning of the current collector and the thickness of the positive electrode and electrolyte, in combination with the electrode kinetics and transport properties.

Results and Discussion

Figure 3 shows the lithium concentration distribution at the surface of the positive electrode particles at time equal to 2700 s during the simulation. The initial concentration of lithium in the positive electrode is 10,000 mol/m^3. During the discharge, as lithium is dissolved on the negative lithium metal electrode, the concentration in the positive electrode increases.

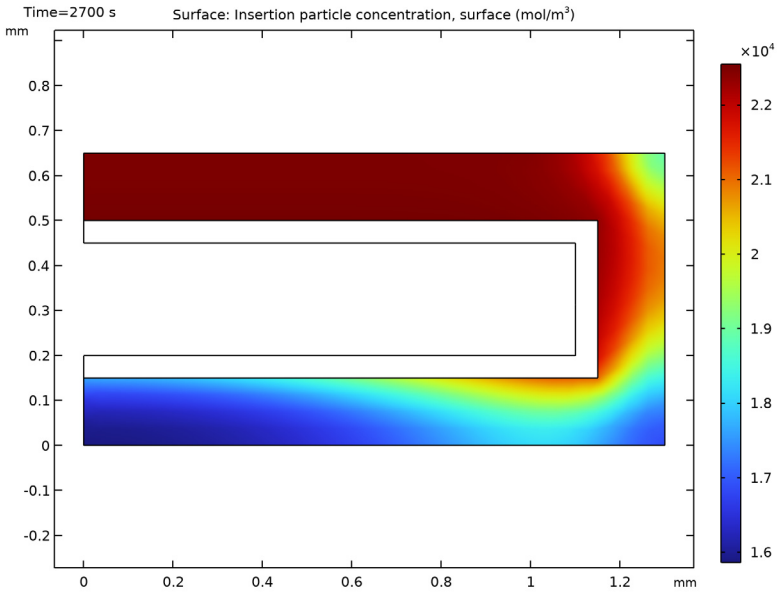


Figure 3: Lithium concentration at the surface of the electrode particles at 2700 s.

The concentration in the positive electrode particles at two selected locations within the positive porous electrode is displayed in Figure 4. Both selections are positioned at the same distance from the electrolyte domain but at different distances from the current collector. The blue line displays the concentration at the location furthest away from the current collector and shows that less discharge has taken place there (concentration lower).

This is consistent with Figure 3.The difference in concentration between the particle center and surface indicate limitations in the lithium transport within the particles.

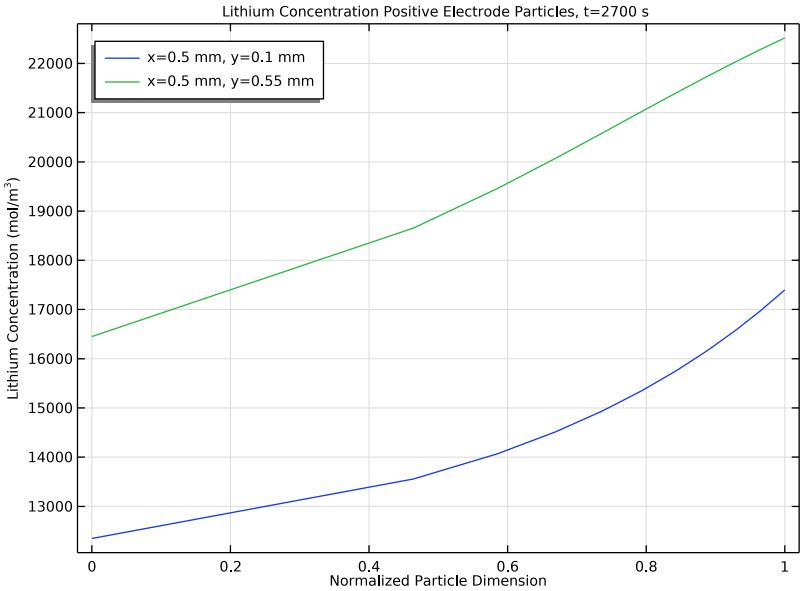


Figure 4: Lithium concentration in the positive electrode particles at two selected positions, (x=0.5 *mm*, *y*=0.1 *mm) and* (x=0.5 *mm*, *y*=0.55 *mm*), *within the model geometry.*

The time-dependent cell voltage predicted by the model during the discharge simulation is shown in Figure 5.

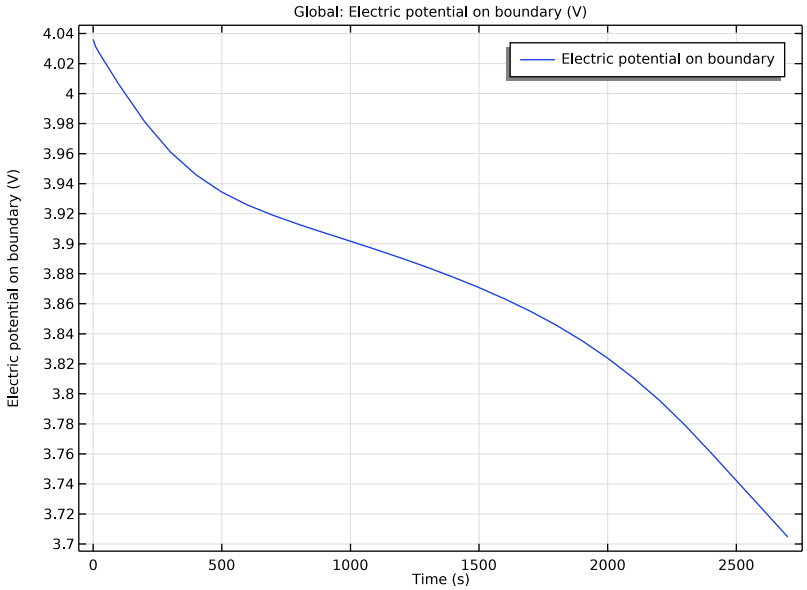


Figure 5: Cell voltage variation during discharge.

Application Library path: `Battery_Design_Module/Batteries,_Lithium-Ion/li_battery_tutorial_2d`

Modeling Instructions

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

NEW

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

MODEL WIZARD

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

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

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces> Time Dependent with Initialization**.

(The **Time Dependent with Initialization study** will perform a time-dependent simulation, using a initialization study step to calculate the initial potentials in the cell.)

6 Click **Done**.

GEOMETRY 1

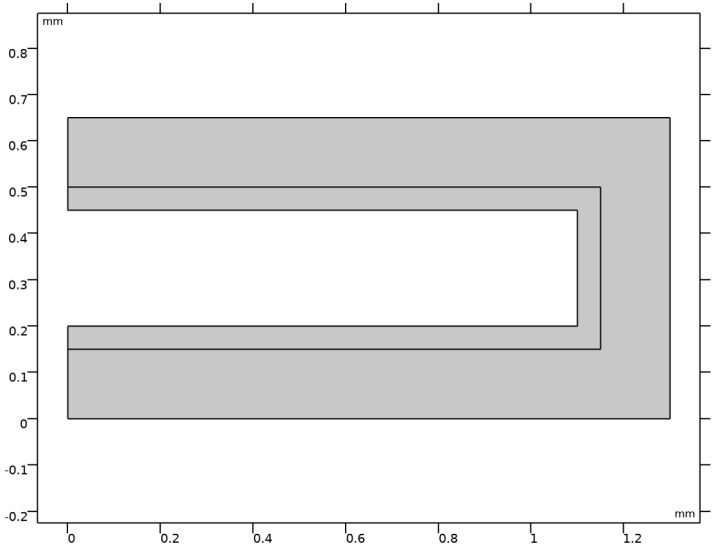
Insert a prepared geometry sequence from a file. After insertion you can study each geometry step in the sequence Appendix — Geometry Modeling Instructions.

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

2 Browse to the model's Application Libraries folder and double-click the file `li_battery_tutorial_2d_geom_sequence.mph`.

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

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



MATERIALS

Use the Battery Material Library to set up the material properties for the electrolyte and electrode materials. By adding the electrolyte material to the model first, this material

becomes the default material for all domains. (In the Materials node, `cEeqref` denotes the maximum lithium concentration in the active material.)

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

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

5 In the tree, select **Battery>Electrodes>LMO, LiMn2O4 Spinel (Positive, Li-ion Battery)**.

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

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

MATERIALS

LMO, LiMn2O4 Spinel (Positive, Li-ion Battery) (mat2)

The first material you added was assigned by default to all domains. Override this default selection by assigning the electrode material to domain 1.

1 Select Domain 1 only.

The LMO material node will now be marked with a small red cross in the model tree, indicating missing material properties. This is expected at this point and will be resolved when setting up the physics for the porous electrode node.

LITHIUM-ION BATTERY (LIION)

An **Electrolyte** node has already been added to the model by default. Now set up the physics in the positive porous electrode.

Porous Electrode 1

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

2 Select Domain 1 only.

The porous electrode contains both an electrode and an electrolyte phase. You therefore need to assign different materials to the different phases. By default, the material properties for each phase will be taken from the material assigned to the domain under **Materials**, which in this case is LMO electrode material. You hence need to set the electrolyte phase material selection manually.

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

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

In this model we will assume that the porous electrode consists of a mix of 40% electrode and 15% inert binder material. The remaining volume is filled up with electrolyte.

5 Locate the **Porous Matrix Properties** section. In the ε_l text field, type `1-0.4-0.15`.

MATERIALS

LMO, LiMn2O4 Spinel (Positive, Li-ion Battery) (mat2)

The small red cross on the LMO material node should now have disappeared in the model tree.

LITHIUM-ION BATTERY (LIION)

Particle Intercalation 1

The **Porous Electrode** has two child nodes added by default. The **Particle Intercalation** node adds an extra dimension to the selected domain, and solves for the diffusion of solid lithium in this extra dimension, assuming spherical particles. Keep the default settings for this node.

Porous Electrode Reaction 1

The **Porous Electrode Reaction** node sets up the equilibrium potential, kinetics and stoichiometry of the lithium insertion reaction occurring at the interface between the electrolyte and electrode phases within the porous matrix. Keep the default settings also for this node.

Electrode Current 1

Finish the model by setting up the boundary conditions. At the positive electrode, set an average current density.

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

2 Select Boundary 10 only.

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

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

5 In the $i_{s,average}$ text field, type `-50[A/m^2]`.

Electrode Surface 1

The negative electrode is a lithium metal foil. This is modeled as a planar electrode using the **Electrode Surface** node.

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

2 Select Boundaries 5, 7, and 12 only.

Electrode Reaction 1

For this reaction, set the equilibrium potential to 0[V].

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

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

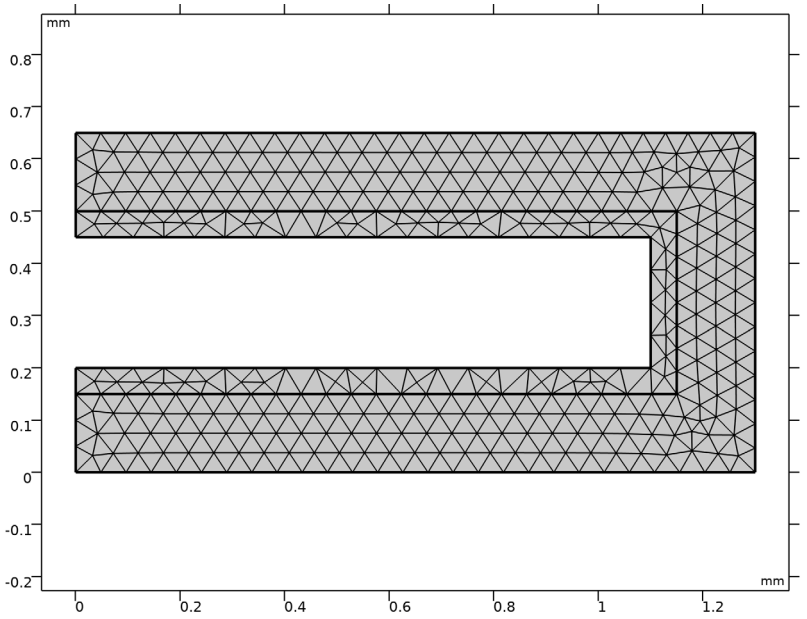
3 From the E_{eq} list, choose **User defined**. Click to expand the **Heat of Reaction** section. From the dE_{eq}/dT list, choose **User defined**.

MESH 1

Use the default physics-controlled mesh for this model.

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Mesh 1** and choose **Build All**.

The generated mesh should look as follows:



STUDY 1

Step 2: Time Dependent

Set up a 2700 s time-dependent solver to store the solution at 10 s intervals during the first 100 s, and 100 s intervals during the last 2600 s.

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. Click **Range** (the small icon to the right of the **Times** text field).
4. In the **Range** dialog box, type `10` in the **Step** text field.
5. In the **Stop** text field, type `100`.
6. Click **Replace**.
7. In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.
8. Click **Range** again.
9. In the **Range** dialog box, type `200` in the **Start** text field.
10. In the **Step** text field, type `100`.
11. In the **Stop** text field, type `2700`.
12. Click **Add**.

    (Alternatively, you may also type in the expression `range(0,10,100) range(200,100,2700)` directly in the **Times** text field.)
13. In the **Home** toolbar, click **Compute**.

RESULTS

Battery Voltage

A plot of the electrode voltage where you set the electrode current condition is created by default. Since you grounded the other electrode this equals the battery voltage during the simulation(Figure 5):

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

Lithium Concentration on Particle Surface

The following steps create a plot of the lithium concentration at the surface of the electrode particles at 2700 s (Figure 3):

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

2 In the **Settings** window for **2D Plot Group**, type `Lithium Concentration on Particle Surface` in the **Label** text field.

Surface 1

1 Right-click **Lithium Concentration on Particle Surface** 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.cs_surface - Insertion particle concentration, surface - mol/m³**.

3 In the **Lithium Concentration on Particle Surface** toolbar, click **Plot**.

Study 1/Solution 1 (3) (sol1)

As mentioned before, the **Particle Intercalation** node adds an extra dimension to the porous electrode domain, and solves for the concentration of solid lithium in this extra dimension. Proceed as follows to create a plot of the lithium concentration in the particles in the positive electrode (Figure 4). In order to do this you need to first create a **Solution** dataset that refers to the extra dimension.

1 In the **Results** toolbar, click **More Datasets** and choose **Solution**.

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

3 From the **Component** list, choose **Extra Dimension from Particle Intercalation 1 (liion_pce1_pin1_xdim)**.

Lithium Concentration in Positive Electrode Particles

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

2 In the **Settings** window for **1D Plot Group**, type `Lithium Concentration in Positive Electrode Particles` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **None**.

Line Graph 1

1 Right-click **Lithium Concentration in Positive Electrode Particles** and choose **Line Graph**.

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

3 From the **Dataset** list, choose **Study 1/Solution 1 (3) (sol1)**.

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

5 Locate the **Selection** section. From the **Selection** list, choose **All domains**.

The `atxd2()` operator is used to specify the `x` and `y` coordinate in the battery geometry.

6 Locate the **y-Axis Data** section. In the **Expression** text field, type `comp1.atxd2(5e-4, 1e-4,liion.cs_pce1)`.

7 Click to expand 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
x=0.5 mm, y=0.1 mm

Line Graph 2

1 Right-click **Line Graph 1** and choose **Duplicate**.

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

3 In the **Expression** text field, type `comp1.atxd2(5e-4,5.5e-4,liion.cs_pce1)`.

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

Legends
x=0.5 mm, y=0.55 mm

Lithium Concentration in Positive Electrode Particles

1 In the **Model Builder** window, click **Lithium Concentration in Positive Electrode Particles**.

2 In the **Settings** window for **1D Plot Group**, click to expand the **Title** section.

3 From the **Title type** list, choose **Manual**.

4 In the **Title** text area, type `Lithium Concentration Positive Electrode Particles, t=2700 s`.

5 Locate the **Plot Settings** section. Select the **x-axis label** check box.

6 In the associated text field, type `Normalized Particle Dimension`.

7 Select the **y-axis label** check box.

8 In the associated text field, type `Lithium Concentration (mol/m<sup>3</sup>)`.

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

10 In the **Lithium Concentration in Positive Electrode Particles** toolbar, click **Plot**.

Appendix — Geometry Modeling Instructions

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

NEW

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

ADD COMPONENT

In the **Home** toolbar, click **Add Component** and choose **2D**.

GEOMETRY 1

1 In the **Settings** window for **Geometry**, locate the **Units** section.

2 From the **Length unit** list, choose **mm**.

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 `1.3`.

4 In the **Height** text field, type `0.65`.

Rectangle 2 (r2)

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 `1.15`.

4 In the **Height** text field, type `0.35`.

5 Locate the **Position** section. In the **y** text field, type `0.15`.

Rectangle 3 (r3)

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 `1.1`.

4 In the **Height** text field, type `0.25`.

5 Locate the **Position** section. In the **y** text field, type `0.2`.

Difference 1 (dif1)

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

2 Select the objects **r1** and **r2** only.

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

4 Find the **Objects to subtract** subsection. Click to select the **Activate Selection** toggle button.

5 Select the object **r3** only.

Point 1 (pt1)

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

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

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

4 In the **y** text field, type `0.65`.

Form Union (fin)

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

2 In the **Settings** window for **Form Union/Assembly**, click  **Build Selected**.