

# Thermal Modeling of a Cylindrical Lithium-Ion Battery in 3D

This example simulates an air-cooled cylindrical 18,650 lithium-ion battery in 3D. A onedimensional cell model is used to model the battery cell chemistry, and a threedimensional model is used to model the temperature in the battery. The two models are coupled by the generated heat source and the average temperature; see Figure 1.

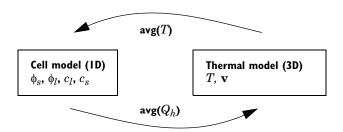


Figure 1: Coupling between the cell and thermal model using the average values for the temperature and generated heat.

The thermal model also includes the flow of the cooling fluid around the battery in a flow compartment, see Figure 2. The fluid flow is allowed to influence the heat transfer rate. This is achieved by using a Nonisothermal Flow multiphysics node. However, the properties of the flow are not assumed to vary with temperature, so a one-way study is used. This approach is significantly less computationally demanding than solving the coupled flow, heat transfer, and electrochemistry problem. The results of this one-way approach will be compared with the coupled solution, in the Results and Discussion section.

# Model Definition

#### CELL MODEL

The cell model is created using the Lithium-Ion Battery interface. A more detailed description on how to set up this type of model can be found in the Application Libraries example 1D Isothermal Lithium-Ion Battery. The cell model consists of the following three domains:

- Negative porous electrode (Li<sub>x</sub>C<sub>6</sub> MCMB, 55 μm)
- Separator (30 μm)
- Positive porous electrode (Li<sub>v</sub>Mn<sub>2</sub>O<sub>4</sub>, 55 μm)

The temperature is set to the mean temperature in the active battery material of the thermal model using a nonlocal integration coupling.

A square wave function is used to set an alternating charge/discharge current at a 7.5C rate with a cycle time of 600 s followed by a relaxing period after 1500 s; see Figure 3. (A 1C rate corresponds to the charge/discharge current required to fully charge or discharge in one hour; 7.5C corresponds to a 7.5 times higher current).

The cell is set to an initial state of charge of 10%.

# THERMAL MODEL

The thermal model is made in 3D using the Heat Transfer in Solids and Fluids interface.

The geometry (see Figure 2) consists of the following domains:

- Active battery material domain (wound sheets of cell material, 65 mm high, radius 9 mm)
- Mandrel (nylon isolator around which the battery cell sheets are wound, 2 mm radius)
- Cylindrical battery connector on top of the battery (steel, 3 mm thick)
- Flow compartment (air)

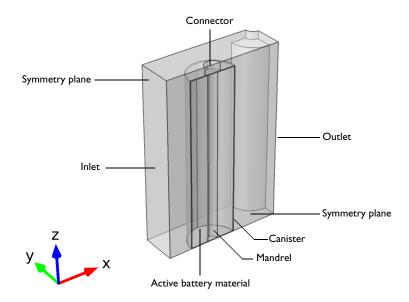


Figure 2: Geometry of the thermal model.

The battery canister (0.25 mm thick) is not included as a domain in the geometry, since the effect of the steel canister on the temperature profile are small, as can be seen in the Thermal Modeling of a Cylindrical Lithium-Ion Battery in 2D model. The heat source term in the active battery material domain is however scaled to account for the lack of heat generation in the current collectors, and for the canister thickness. This scaled heat source is obtained by multiplying the volumetric heat source from the 1D Li-ion battery model by two factors. The first factor is the fraction of the total 1D model in which heat is generated. That is the sum of lengths of the negative electrode, separator and the positive electrode, divided the total cell length, which also includes the lengths of the two current collectors. The second factor is the fraction of the total 3D cylindrical cell geometry in which heat is generated. The volume in which heat is generated is the total volume of the cell (which includes both the homogenized wound layers of the battery material, the central mandrel and the outer can), minus the volume of the mandrel and the volume of the outer can. This heat source is then divided by the total volume of battery material, which is the difference between the total cell volume and the mandrel volume. Thus, the following expression for the 3D heat source is obtained:

$$Q_{h, 3D} = Q_{h, 1D} \frac{L_{\text{neg}} + L_{\text{sep}} + L_{\text{pos}} ((r_{\text{batt}} - d_{\text{can}})^2 - r_{\text{mandrel}}^2)(h_{\text{batt}} - 2d_{\text{can}})}{(r_{\text{batt}}^2 - r_{\text{mandrel}}^2)h_{\text{batt}}}$$

The battery is placed in a battery pack consisting of a matrix of batteries.

The thermal conductivity in the active battery material is anisotropic due to the spiral winding of the battery cell layers. The thermal conductivity, density, heat capacity and heat source in the battery are set up in the same way as in the Thermal Modeling of a Cylindrical Lithium-Ion Battery in 2D model. A cylindrical coordinate system is added in the model in order to handle the orthotropic thermal conductivity in the active material.

The heat source based in the active battery domain is set to the average of the generated heat in cell model using a nonlocal coupling integration variable. At the inlet boundary a temperature of 298.15 K is specified whereas an outflow condition is applied at the outlet. All other external boundaries are thermally isolated. The initial temperature of the battery is 298.15 K.

For the flow, an inlet velocity of 0.1 m/s is applied at the inlet, and a pressure of 1 atm is set at the outlet. Symmetry boundary conditions are applied to the symmetry planes. No Slip conditions are applied to the battery walls.

The problem is solved in three steps. In the first step the steady state flow at 298.15 K is solved for. The second step solves for the potentials in battery model at t = 0. The third step is a time-dependent study of the full problem, where the steady state solution from

the first two steps are used to set the initial values for the potentials. The velocity and pressure of the cooling gas is assumed to be almost unaffected by the heat transfer from the battery.

# Results and Discussion

Figure 3 shows the cell potential and the load cycle current.

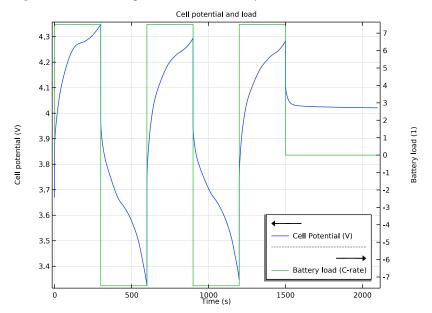


Figure 3: Cell potential and current load.

Figure 4 shows the minimum, maximum, and average temperatures of the battery during the simulation. The difference in heating rate between charge and discharge is due to the difference in entropy change for the charge and discharge reactions (set by the dEeq/dT parameter).

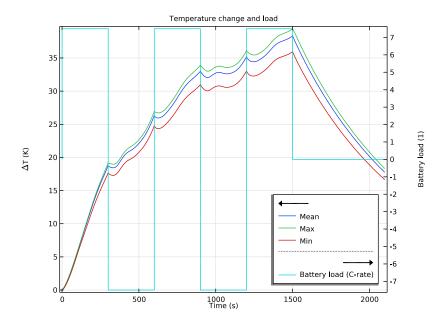


Figure 4: Minimum, mean, and maximum temperature.

Figure 5 shows the temperature in the battery and streamlines for the flow at 1500 s. The temperature maximum is located in the active battery material toward the thermally isolated end.

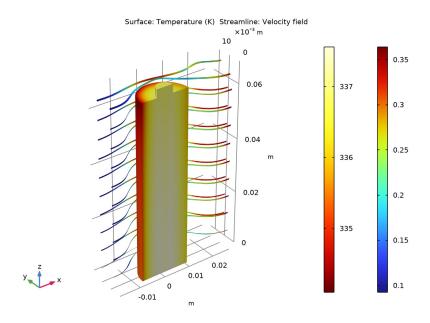


Figure 5: Temperature and flow at t=1500 s.

Figure 6 shows the difference in battery temperature and airflow streamlines between the coupled solution and the one-way solution. The differences are calculated using a Join dataset. In this case, the one-way solution is very similar to the coupled one, since only the fluid viscosity is temperature-dependent. The details of the flow pattern do change, but with a magnitude that is only a few percent of the total fluid flow velocity. The one-way calculation completes in a fraction of the time that the coupled calculation requires. This usage of the Nonisothermal Flow multiphysics feature in a one-way study to compute flow, heat, and the battery electrochemistry illustrates one key simplification that might be used in many thermal battery models. At the same time, checking the assumption is simple.

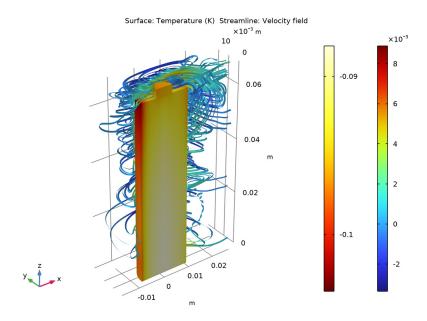


Figure 6: Differences in battery temperature and fluid flow streamlines between the coupled and one-way solutions after 2100 s.

# Notes About the COMSOL Implementation

To improve to convergence of the time-dependent solver, the function nojac() is used when setting up the nonlocal couplings for the average temperature and heat source.

Application Library path: Battery\_Design\_Module/Thermal\_Management/ li battery thermal 3d

# Modeling Instructions

# APPLICATION LIBRARIES

- I From the File menu, choose Application Libraries.
- 2 In the Application Libraries window, select Battery Design Module>Thermal Management> li\_battery\_I d\_for\_thermal\_models in the tree.

3 Click Open.

#### ADD COMPONENT

In the Home toolbar, click Add Component and choose 3D.

#### ADD PHYSICS

- I In the Home toolbar, click open the Add Physics window.
- 2 Go to the Add Physics window.
- 3 In the tree, select Fluid Flow>Single-Phase Flow>Laminar Flow (spf).
- 4 Click Add to Component 2 in the window toolbar.
- 5 In the tree, select Heat Transfer>Heat Transfer in Solids and Fluids (ht).
- 6 Click Add to Component 2 in the window toolbar.
- 7 In the Home toolbar, click of Add Physics to close the Add Physics window.

#### MULTIPHYSICS

Add a Nonisothermal flow multiphysics node to set up the velocity in heat transfer and to account for the multiphysics stabilization.

Nonisothermal Flow I (nitfl)

In the Physics toolbar, click Aultiphysics Couplings and choose Domain> Nonisothermal Flow.

#### **GLOBAL DEFINITIONS**

# Parameters 1

- I In the Model Builder window, under Global Definitions click Parameters I.
- 2 In the Settings window for Parameters, locate the Parameters section.
- **3** In the table, enter the following settings:

Name	Expression	Value	Description	
h_connector	3[mm]	0.003 m	Connector height	
r_connector	3[mm]	0.003 m	Connector radius	
s_inlet	2*r_batt	0.018 m	Length of inlet flow region	
s_matrix	3*r_batt	0.027 m	Battery-battery distance in matrix	
V_in	0.1[m/s]	0.1 m/s	Inlet velocity	
t	0	0	Time parameter in initialization study step	

#### **GEOMETRY 2**

Cvlinder I (cvl I)

- I In the Geometry toolbar, click Cylinder.
- 2 In the Settings window for Cylinder, locate the Size and Shape section.
- 3 In the Radius text field, type r\_batt.
- 4 In the Height text field, type h batt.
- 5 Click | Build Selected.
- 6 Click the Transparency button in the Graphics toolbar.

Cylinder 2 (cyl2)

- I In the **Geometry** toolbar, click **Cylinder**.
- 2 In the Settings window for Cylinder, locate the Size and Shape section.
- 3 In the Radius text field, type r\_mandrel.
- 4 In the **Height** text field, type h batt.

Cylinder 3 (cyl3)

- I In the **Geometry** toolbar, click **Cylinder**.
- 2 In the Settings window for Cylinder, locate the Size and Shape section.
- 3 In the Radius text field, type r\_connector.
- 4 In the Height text field, type h connector.
- 5 Locate the **Position** section. In the z text field, type h batt.
- 6 Click | Build Selected.

Union I (uni I)

- I In the Geometry toolbar, click Booleans and Partitions and choose Union.
- 2 Click in the **Graphics** window and then press Ctrl+A to select all objects.
- 3 In the Settings window for Union, click **Build Selected**.

Block I (blk I)

- I In the Geometry toolbar, click Block.
- 2 In the Settings window for Block, locate the Size and Shape section.
- 3 In the Width text field, type 2\*r batt.
- 4 In the **Depth** text field, type r batt.
- 5 In the **Height** text field, type h\_batt+h\_connector.
- 6 Locate the **Position** section. In the **x** text field, type -r batt.

7 Click Pauld Selected.

Intersection I (intl)

- I In the Geometry toolbar, click Booleans and Partitions and choose Intersection.
- 2 Click in the **Graphics** window and then press Ctrl+A to select both objects.
- 3 In the Settings window for Intersection, click 📳 Build Selected.

Block 2 (blk2)

- I In the Geometry toolbar, click Block.
- 2 In the Settings window for Block, locate the Size and Shape section.
- **3** In the **Width** text field, type s\_inlet+s\_matrix.
- 4 In the **Depth** text field, type s\_matrix/2.
- 5 In the **Height** text field, type h\_batt-5[mm].
- 6 Locate the Position section. In the x text field, type -s\_inlet.
- 7 Click Pauld Selected.

Block 3 (blk3)

- I In the Geometry toolbar, click Block.
- 2 In the Settings window for Block, locate the Size and Shape section.
- **3** In the **Width** text field, type s\_inlet+s\_matrix.
- 4 In the **Depth** text field, type s matrix/2.
- 5 In the **Height** text field, type h connector+5[mm].
- 6 Locate the Position section. In the x text field, type -s\_inlet.
- 7 In the z text field, type h batt-5[mm].
- 8 Click | Build Selected.

Cylinder 4 (cyl4)

- I In the **Geometry** toolbar, click **Cylinder**.
- 2 In the Settings window for Cylinder, locate the Size and Shape section.
- 3 In the Radius text field, type r\_batt.
- 4 In the **Height** text field, type h batt.
- **5** Locate the **Position** section. In the **x** text field, type **s** matrix.
- 6 In the y text field, type s\_matrix/2.
- 7 Click | Build Selected.

# Cylinder 5 (cyl5)

- I In the Geometry toolbar, click ( Cylinder.
- 2 In the Settings window for Cylinder, locate the Size and Shape section.
- 3 In the Radius text field, type r\_connector.
- 4 In the **Height** text field, type h\_connector.
- **5** Locate the **Position** section. In the **x** text field, type **s** matrix.
- 6 In the y text field, type s\_matrix/2.
- 7 In the z text field, type h\_batt.
- 8 Click Pauld Selected.

# Difference I (dif1)

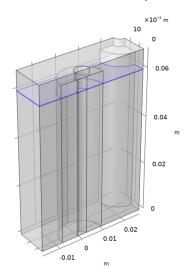
- I In the Geometry toolbar, click Booleans and Partitions and choose Difference.
- 2 Select the objects blk2, blk3, and int1 only.
- 3 In the Settings window for Difference, locate the Difference section.
- **4** Click to select the **Activate Selection** toggle button for **Objects to subtract**.
- **5** Select the objects **cyl4** and **cyl5** only.
- 6 Click | Build Selected.

# Mesh Control Faces 1 (mcf1)

- I In the Geometry toolbar, click \times \text{Virtual Operations} and choose Mesh Control Faces.
- 2 On the object fin, select Boundaries 6, 15, and 26 only.

It might be easier to select the domains by using the **Selection List** window. To open this window, in the Home toolbar click Windows and choose Selection List. (If you are running the cross-platform desktop, you find **Windows** in the main menu.)

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





# **DEFINITIONS (COMP2)**

# Flow Compartment

- I In the **Definitions** toolbar, click **\( \big|\_{\bigsip} Explicit. \)**
- 2 In the Settings window for Explicit, type Flow Compartment in the Label text field.
- **3** Select Domain 1 only.

# Active Battery Material

- I In the **Definitions** toolbar, click 🔓 **Explicit**.
- 2 In the **Settings** window for **Explicit**, type Active Battery Material in the **Label** text field.
- **3** Select Domain 2 only.

# **Battery Connector**

- I In the **Definitions** toolbar, click 堶 **Explicit**.
- 2 In the Settings window for Explicit, type Battery Connector in the Label text field.
- **3** Select Domain 3 only.

#### Mandrel

- I In the **Definitions** toolbar, click **\( \frac{1}{2} \) Explicit**.
- 2 In the Settings window for Explicit, type Mandrel in the Label text field.

**3** Select Domain 4 only.

#### Inlet

- I In the **Definitions** toolbar, click **\( \frac{1}{2} \) Explicit**.
- 2 In the Settings window for Explicit, type Inlet in the Label text field.
- 3 Locate the Input Entities section. From the Geometric entity level list, choose Boundary.
- 4 Select Boundary 1 only.

#### Outlet

- 2 In the Settings window for Explicit, type Outlet in the Label text field.
- 3 Locate the Input Entities section. From the Geometric entity level list, choose Boundary.
- 4 Select Boundary 26 only.

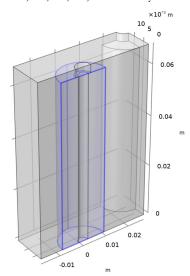
# Symmetry planes

- I In the **Definitions** toolbar, click **\( \frac{1}{2} \) Explicit**.
- 2 In the Settings window for Explicit, type Symmetry planes in the Label text field.
- 3 Locate the Input Entities section. From the Geometric entity level list, choose Boundary.
- 4 Select Boundaries 2, 5, and 22 only.

#### Can

- I In the **Definitions** toolbar, click **\( \frac{1}{2} \) Explicit**.
- 2 In the Settings window for Explicit, type Can in the Label text field.
- 3 Locate the Input Entities section. From the Geometric entity level list, choose Boundary.

**4** Select Boundaries 7–9, 12, 16, 17, and 20 only.



# Average I (aveob I)

Define a nonlocal coupling for the average temperature in the active battery material of the 3D thermal model to use in the 1D battery model.

- I In the **Definitions** toolbar, click Nonlocal Couplings and choose Average.
- 2 In the Settings window for Average, locate the Source Selection section.
- **3** From the Selection list, choose Active Battery Material.

# SHARED PROPERTIES

Now go to Component 1 (the 1D battery model) and define a model input for the average temperature from the 3D thermal model. Use no jac () to improve the time-dependent solver convergence.

#### Model Input 1

- I In the Model Builder window, expand the Component I (compl)>Definitions> Shared Properties node, then click Model Input 1.
- 2 In the Settings window for Model Input, locate the Definition section.
- 3 In the text field, type nojac(comp2.aveop1(comp2.T)).

#### **DEFINITIONS (COMPI)**

Average 2 (aveop2)

- I In the **Definitions** toolbar, click **Monlocal Couplings** and choose **Average**. This average operator defined in Component 1 for the 1D battery cell model is used for calculating a mean heat source for coupling to the 3D heat transfer model.
- 2 In the Settings window for Average, locate the Source Selection section.
- 3 From the Selection list, choose All domains.

# **DEFINITIONS (COMP2)**

Now go to Component 2 (the 3D heat transfer model) and define a variable for the heat source. Use nojac() to improve the time-dependent solver convergence.

- I In the Model Builder window, under Component 2 (comp2) click Definitions.
- 2 Click the Component 2 node.

Variables 2

- I In the **Definitions** toolbar, click **a= Local Variables**.
- 2 In the Settings window for Variables, locate the Variables section.
- **3** In the table, enter the following settings:

Name	Expression	Unit	Description
Qh	<pre>nojac(comp1.aveop2(comp1 .liion.Qh))*(L_neg+ L_sep+L_pos)/L_batt* ((r_batt-d_can)^2- r_mandrel^2)*(h_batt-d_can*2)/((r_batt^2-r_mandrel^2)*h_batt)</pre>	W/m³	Average heat source from 1d battery model
r	sqrt(x^2+y^2)	m	Radius

#### **DEFINITIONS (COMPI)**

Point Probe Expression I (CellVoltageProbe)

- I In the Model Builder window, expand the Domain Point Probe I node, then click Point Probe Expression I (CellVoltageProbe).
- 2 In the Settings window for Point Probe Expression, click to expand the Table and Window Settings section.
- 3 Click + Add Plot Window.

# DEFINITIONS (COMP2)

In the Model Builder window, under Component 2 (comp2) click Definitions.

#### Domain Probe I (dom I)

- I In the Definitions toolbar, click Probes and choose Domain Probe.
- 2 In the Settings window for Domain Probe, type MeanT in the Variable name text field.
- **3** Locate the **Source Selection** section. From the **Selection** list, choose **Active Battery Material**.
- **4** Locate the **Expression** section. In the **Expression** text field, type T-T\_inlet.
- 5 Click to expand the Table and Window Settings section. From the Plot window list, choose Probe Plot 1.

# Domain Probe 2 (dom2)

- I In the **Definitions** toolbar, click **Probes** and choose **Domain Probe**.
- 2 In the Settings window for Domain Probe, locate the Probe Type section.
- 3 From the Type list, choose Maximum.
- 4 In the Variable name text field, type MaxT.
- 5 Locate the Source Selection section. From the Selection list, choose Active Battery Material.
- **6** Locate the **Expression** section. In the **Expression** text field, type T-T inlet.
- 7 Locate the Table and Window Settings section. From the Plot window list, choose Probe Plot 1.

#### Domain Probe 3 (dom3)

- I In the **Definitions** toolbar, click Probes and choose **Domain Probe**.
- 2 In the Settings window for Domain Probe, locate the Probe Type section.
- **3** From the **Type** list, choose **Minimum**.
- 4 In the Variable name text field, type MinT.
- **5** Locate the **Source Selection** section. From the **Selection** list, choose **Active Battery Material**.
- **6** Locate the **Expression** section. In the **Expression** text field, type T-T\_inlet.
- 7 Locate the Table and Window Settings section. From the Plot window list, choose Probe Plot 1.

#### ADD MATERIAL

I In the Home toolbar, click **4** Add Material to open the Add Material window.

- 2 Go to the Add Material window.
- 3 In the tree, select Built-in>Steel AISI 4340.
- **4** Click **Add to Component** in the window toolbar.
- 5 In the tree, select Built-in>Nylon.
- **6** Click **Add to Component** in the window toolbar.
- 7 In the tree, select Built-in>Air.
- **8** Click **Add to Component** in the window toolbar.
- 9 In the tree, select Built-in>Steel AISI 4340.
- **10** Click **Add to Component** in the window toolbar.
- II In the Home toolbar, click **‡ Add Material** to close the **Add Material** window.

#### MATERIALS

Steel AISI 4340 (mat4)

- I In the Model Builder window, under Component 2 (comp2)>Materials click Steel AISI 4340 (mat4).
- 2 In the Settings window for Material, locate the Geometric Entity Selection section.
- 3 From the Selection list, choose Battery Connector.

Nylon (mat5)

- I In the Model Builder window, click Nylon (mat5).
- 2 In the Settings window for Material, locate the Geometric Entity Selection section.
- 3 From the Selection list, choose Mandrel.

Air (mat6)

- I In the Model Builder window, click Air (mat6).
- 2 In the Settings window for Material, locate the Geometric Entity Selection section.
- 3 From the Selection list, choose Flow Compartment.

Steel AISI 4340.1 (mat7)

- I In the Model Builder window, click Steel AISI 4340.1 (mat7).
- 2 In the Settings window for Material, locate the Geometric Entity Selection section.
- 3 From the Geometric entity level list, choose Boundary.
- 4 From the Selection list, choose Can.

#### **DEFINITIONS (COMP2)**

Add a cylindrical coordinate system to handle the orthotropic thermal conductivity in the active battery material.

Cylindrical System 2 (sys2)

In the Definitions toolbar, click  $\bigvee_{x}^{z}$  Coordinate Systems and choose Cylindrical System.

#### HEAT TRANSFER IN SOLIDS AND FLUIDS (HT)

#### Solid 2

- I In the Model Builder window, under Component 2 (comp2) right-click Heat Transfer in Solids and Fluids (ht) and choose Solid.
- 2 In the Settings window for Solid, locate the Domain Selection section.
- 3 From the Selection list, choose Active Battery Material.
- 4 Locate the Coordinate System Selection section. From the Coordinate system list, choose Cylindrical System 2 (sys2).
- **5** Locate the **Heat Conduction, Solid** section. From the k list, choose **User defined**. From the list, choose **Diagonal**.
- **6** In the *k* table, enter the following settings:

kT_batt_r	0	0
0	kT_batt_ang	0
0	0	kT_batt_ang

- 7 Locate the Thermodynamics, Solid section. From the  $\rho$  list, choose User defined. In the associated text field, type rho\_batt.
- 8 From the  $C_p$  list, choose User defined. In the associated text field, type  ${\tt Cp\_batt.}$

#### Heat Source 1

- I In the Physics toolbar, click Domains and choose Heat Source.
- 2 In the Settings window for Heat Source, locate the Domain Selection section.
- 3 From the Selection list, choose Active Battery Material.
- **4** Locate the **Heat Source** section. In the  $Q_0$  text field, type Qh.

#### LAMINAR FLOW (SPF)

- I In the Model Builder window, under Component 2 (comp2) click Laminar Flow (spf).
- 2 In the Settings window for Laminar Flow, locate the Domain Selection section.
- 3 From the Selection list, choose Flow Compartment.

#### HEAT TRANSFER IN SOLIDS AND FLUIDS (HT)

#### Fluid 1

- I In the Model Builder window, under Component 2 (comp2)> Heat Transfer in Solids and Fluids (ht) click Fluid 1.
- 2 In the Settings window for Fluid, locate the Domain Selection section.
- 3 From the Selection list, choose Flow Compartment.

#### Temberature I

- I 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 Inlet.
- **4** Locate the **Temperature** section. In the  $T_0$  text field, type T\_inlet.

#### Outflow I

- I In the Physics toolbar, click **Boundaries** and choose **Outflow**.
- 2 In the Settings window for Outflow, locate the Boundary Selection section.
- 3 From the Selection list, choose Outlet.

# LAMINAR FLOW (SPF)

In the Model Builder window, under Component 2 (comp2) click Laminar Flow (spf).

#### Outlet I

- I In the Physics toolbar, click **Boundaries** and choose **Outlet**.
- 2 In the Settings window for Outlet, locate the Boundary Selection section.
- 3 From the Selection list, choose Outlet.
- 4 Locate the Pressure Conditions section. Select the Normal flow check box.

#### Inlet 1

- I In the Physics toolbar, click **Boundaries** and choose Inlet.
- 2 In the Settings window for Inlet, locate the Boundary Selection section.
- **3** From the **Selection** list, choose **Inlet**.
- **4** Locate the **Velocity** section. In the  $U_0$  text field, type  $V_i$ n.

#### Symmetry I

- I In the Physics toolbar, click **Boundaries** and choose Symmetry.
- 2 In the Settings window for Symmetry, locate the Boundary Selection section.
- 3 From the Selection list, choose Symmetry planes.

#### HEAT TRANSFER IN SOLIDS AND FLUIDS (HT)

- I In the Model Builder window, under Component 2 (comp2) click Heat Transfer in Solids and Fluids (ht).
- 2 In the Settings window for Heat Transfer in Solids and Fluids, locate the Physical Model section.
- **3** In the  $T_{\text{ref}}$  text field, type T\_init.

#### Initial Values 1

- I In the Model Builder window, under Component 2 (comp2)> Heat Transfer in Solids and Fluids (ht) click Initial Values I.
- 2 In the Settings window for Initial Values, locate the Initial Values section.
- **3** In the *T* text field, type T\_init.

#### MESH 2

#### Size 1

- I In the Model Builder window, under Component 2 (comp2) right-click Mesh 2 and choose Size.
- 2 In the Settings window for Size, locate the Geometric Entity Selection section.
- 3 From the Geometric entity level list, choose Domain.
- 4 From the Selection list, choose Flow Compartment.
- 5 Locate the Element Size section. From the Calibrate for list, choose Fluid dynamics.
- 6 From the Predefined list, choose Fine.

#### Swebt I

- I In the Mesh toolbar, click A Swept.
- 2 In the Settings window for Swept, locate the Domain Selection section.
- 3 From the Geometric entity level list, choose Domain.
- **4** Select Domains 1, 2, and 4 only.
- 5 Click to expand the Sweep Method section. From the Face meshing method list, choose Triangular (generate prisms).

#### Distribution I

- I Right-click Swept I and choose Distribution.
- 2 In the Settings window for Distribution, locate the Distribution section.
- 3 In the Number of elements text field, type 10.
- 4 Click Build Selected.

# Free Tetrahedral I

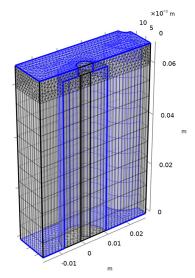
- I In the Mesh toolbar, click Free Tetrahedral.
- 2 In the Settings window for Free Tetrahedral, click to expand the Control Entities section.
- 3 Clear the Smooth across removed control entities check box.
- 4 Click Build Selected.

# Boundary Layers 1

- I In the Mesh toolbar, click Boundary Layers.
- 2 In the Settings window for Boundary Layers, locate the Geometric Entity Selection section.
- 3 From the Geometric entity level list, choose Domain.
- 4 From the Selection list, choose Flow Compartment.

# Boundary Layer Properties

- I In the Model Builder window, click Boundary Layer Properties.
- **2** Select Boundaries 3, 4, 7, 9, 11, 19, 20, and 23–25 only.





- 3 In the Settings window for Boundary Layer Properties, locate the Layers section.
- 4 In the Number of layers text field, type 2.
- 5 From the Thickness specification list, choose First layer.
- 6 In the Thickness text field, type 2e-4.

# Boundary Layers 1

- I In the Model Builder window, click Boundary Layers I.
- 2 In the Settings window for Boundary Layers, click to expand the Transition section.
- 3 Clear the Smooth transition to interior mesh check box.
- 4 Click Build Selected.

#### ADD STUDY

- I 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 Model Builder window, click the root node.
- 6 In the Home toolbar, click Add Study to close the Add Study window.

#### STUDY I

Step 1: Stationary

- I In the Settings window for Stationary, locate the Physics and Variables Selection section.
- 2 In the table, clear the Solve for check boxes for Lithium-Ion Battery (liion) and Heat Transfer in Solids and Fluids (ht).
- 3 In the table, clear the Solve for check box for Nonisothermal Flow I (nitfl).

Step 2: Current Distribution Initialization

In the Study toolbar, click Study Steps and choose Other>

#### **Current Distribution Initialization.**

Step 3: Time Dependent

I In the Study toolbar, click Study Steps and choose Time Dependent> Time Dependent.

The square wave current density cycle we are applying results in sharp transients. However, as we know at which times the current density is changed, we can combine a strict time stepping with custom values of times to solve for. Then, we provide a hint for the solver about which times are most critical to resolve well. Doing so aids convergence.

- 2 In the Settings window for Time Dependent, locate the Study Settings section.
- **3** In the **Output times** text field, type 0 299.95 300 599.95 600 899.95 900 1199.95 1200 1499.95 1500 2100.

4 Locate the Physics and Variables Selection section. In the table, clear the Solve for check box for Laminar Flow (spf).

Solution I (soll)

By making a few further changes to the time-dependent solver, we can improve convergence. The strict time stepping is chosen to allow us to control what times the solver solves for. As we know that the model starts with a step in current density at time 0, manually selecting a small initial step size helps convergence. Without it, the solver will start with a larger step size (the default 0.1% of the end time) where it cannot find convergence. Using the Automatic (Newton) solver is suitable for the nonlinear electrochemistry problem. Moving the segregated step for the electrochemistry problem to the top can also yield a small additional speedup, since the 1D electrochemical component is what yields the heat source.

- I In the Study toolbar, click Show Default Solver.
- 2 In the Model Builder window, expand the Solution I (soll) node, then click Time-Dependent Solver I.
- 3 In the Settings window for Time-Dependent Solver, click to expand the Time Stepping section.
- 4 From the Steps taken by solver list, choose Strict.
- 5 Click to expand the Advanced section. Locate the Time Stepping section. Find the Algebraic variable settings subsection. From the Consistent initialization list, choose Off.
- 6 In the Model Builder window, expand the Study I>Solver Configurations> Solution I (soll)>Time-Dependent Solver I>Segregated I node, then click **Battery Current Distribution.**
- 7 In the Settings window for Segregated Step, click to expand the Method and Termination section.
- 8 From the Nonlinear method list, choose Automatic (Newton).
- 9 Right-click Study I>Solver Configurations>Solution I (sol1)>Time-Dependent Solver I> Segregated I>Battery Current Distribution and choose Move Up.
- **10** In the **Model Builder** window, click **Study 1**.
- II In the Settings window for Study, locate the Study Settings section.
- 12 Clear the Generate default plots check box.
- **13** In the **Study** toolbar, click **Compute**.

#### RESULTS

# Probe Plot Group 1

- I In the Model Builder window, expand the Results>Probe Plot Group I node, then click Probe Plot Group 1.
- 2 In the Settings window for ID Plot Group, click to expand the Title section.
- 3 From the Title type list, choose Manual.
- 4 In the Title text area, type Cell potential and load.
- 5 Locate the Plot Settings section. Select the Two y-axes check box.
- 6 Select the y-axis label check box. In the associated text field, type Cell potential (V).
- 7 Select the Secondary y-axis label check box. In the associated text field, type Battery load (1).
- 8 Locate the Legend section. From the Position list, choose Lower right.

#### Cell Potential (V)

- I In the Model Builder window, under Results>Probe Plot Group I click Probe Table Graph 1.
- 2 In the Settings window for Table Graph, type Cell Potential (V) in the Label text field.
- 3 Click to expand the **Legends** section. Select the **Show legends** check box.
- **4** Find the **Include** subsection. Select the **Label** check box.
- 5 Clear the Headers check box.
- 6 Right-click Cell Potential (V) and choose Duplicate.

# Battery load (C-rate)

- I In the Model Builder window, click Cell Potential (V) I.
- 2 In the Settings window for Table Graph, locate the Data section.
- 3 In the Columns list, select i\_app/i\_IC.
- 4 Locate the y-Axis section. Select the Plot on secondary y-axis check box.
- 5 In the Label text field, type Battery load (C-rate).
- 6 In the Probe Plot Group I toolbar, click **Plot**.

# Probe Plot Group 2

- I In the Model Builder window, expand the Results>Probe Plot Group 2 node, then click Probe Plot Group 2.
- 2 In the Settings window for ID Plot Group, locate the Title section.

- 3 From the Title type list, choose Manual.
- 4 In the Title text area, type Temperature change and load.
- **5** Locate the **Plot Settings** section. Select the **Two y-axes** check box.
- 6 Select the y-axis label check box. In the associated text field, type \DELTA T (K).
- 7 Select the Secondary y-axis label check box. In the associated text field, type Battery load (1).
- 8 Locate the Legend section. From the Position list, choose Lower right.

#### Probe Table Graph 1

- I In the Model Builder window, click Probe Table Graph I.
- 2 In the Settings window for Table Graph, locate the Data section.
- 3 In the Columns list, choose T-T\_inlet (K), Domain Probe I, T-T\_inlet (K), Domain Probe 2, and T-T\_inlet (K), Domain Probe 3.
- 4 Locate the Legends section. From the Legends list, choose Manual.
- **5** In the table, enter the following settings:

Legends	
Mean	
Max	
Min	

6 In the Probe Plot Group 2 toolbar, click  **Plot**.

# Battery load (C-rate)

- I In the Model Builder window, right-click Probe Plot Group 2 and choose Table Graph.
- 2 In the Settings window for Table Graph, type Battery load (C-rate) in the Label text field.
- 3 Locate the Data section. From the Plot columns list, choose Manual.
- 4 In the Columns list, select i\_app/i\_IC.
- **5** Locate the **y-Axis** section. Select the **Plot on secondary y-axis** check box.
- **6** Locate the **Legends** section. Select the **Show legends** check box.
- 7 Find the **Include** subsection. Select the **Label** check box.
- 8 Clear the Headers check box.

# Temberature

- I In the Model Builder window, under Results>Probe Plot Group 2 click Probe Table Graph 1.
- 2 In the Settings window for Table Graph, type Temperature in the Label text field.
- 3 In the Probe Plot Group 2 toolbar, click Plot.
- 4 Click the **Zoom Extents** button in the **Graphics** toolbar.

# **DEFINITIONS (COMP2)**

In the Model Builder window, under Component 2 (comp2)>Definitions click Selections.

# Battery Surface

- I In the **Definitions** toolbar, click **\( \) Adjacent**.
- 2 In the Settings window for Adjacent, locate the Input Entities section.
- 3 Under Input selections, click + Add.
- 4 In the Add dialog box, in the Input selections list, choose Active Battery Material, Battery Connector, and Mandrel.
- 5 Click OK.
- 6 In the Settings window for Adjacent, locate the Output Entities section.
- 7 Select the Interior boundaries check box.
- 8 In the Label text field, type Battery Surface.

#### RESULTS

Study I/Solution I (9) (soll)

- I 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 Component 2 (comp2).

#### Selection

- I Right-click Study I/Solution I (9) (soll) and choose Selection.
- 2 In the Settings window for Selection, locate the Geometric Entity Selection section.
- 3 From the Geometric entity level list, choose Boundary.
- 4 From the Selection list, choose Battery Surface.
- 5 Click the Transparency button in the Graphics toolbar.

# Temberature and flow

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

- 2 In the Settings window for 3D Plot Group, type Temperature and flow in the Label text
- 3 Locate the Plot Settings section. Clear the Plot dataset edges check box.
- 4 Locate the Data section. From the Dataset list, choose None.

# Surface I

- I Right-click Temperature and flow and choose Surface.
- 2 In the Settings window for Surface, locate the Data section.
- 3 From the Dataset list, choose Study I/Solution I (9) (soll).
- 4 From the Time (s) list, choose 1500 (2).
- **5** Locate the **Expression** section. In the **Expression** text field, type T.
- 6 Locate the Coloring and Style section. Click Change Color Table.
- 7 In the Color Table dialog box, select Thermal>Thermal in the tree.
- 8 Click OK.
- 9 In the Temperature and flow toolbar, click Plot.

#### Streamline 1

- I In the Model Builder window, right-click Temperature and flow and choose Streamline.
- 2 In the Settings window for Streamline, locate the Data section.
- 3 From the Dataset list, choose Study I/Solution I (9) (soll).
- 4 From the Time (s) list, choose 1500 (2).
- 5 Click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component 2 (comp2)>Laminar Flow>Velocity and pressure>u,v,w -Velocity field.
- 6 Locate the Streamline Positioning section. From the Positioning list, choose On selected boundaries.
- 7 Locate the Selection section. From the Selection list, choose Inlet.
- 8 Locate the Coloring and Style section. Find the Line style subsection. From the Type list, choose Ribbon.

# Color Expression 1

- I Right-click Streamline I and choose Color Expression.
- 2 In the Settings window for Color Expression, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component 2 (comp2)> Laminar Flow>Velocity and pressure>spf.U - Velocity magnitude - m/s.

- 3 In the Temperature and flow toolbar, click Plot.
- 4 Click the **Zoom Extents** button in the **Graphics** toolbar.

#### Load cycle

- I In the Model Builder window, under Results right-click Probe Plot Group I and choose
- 2 In the Rename ID Plot Group dialog box, type Load cycle in the New label text field.
- 3 Click OK.

# Temperature vs. Time

- I In the Model Builder window, right-click Probe Plot Group 2 and choose Rename.
- 2 In the Rename ID Plot Group dialog box, type Temperature vs. Time in the New label text field.
- 3 Click OK.

In order to simulate a bidirectionally coupled approach for flow and temperature computation, a new study can be set up as above, but with Laminar Flow being solved for in the **Time Dependent** study step. A plot comparing the bidirectionally and unidirectionally coupled approaches can be created using **Join** datasets to evaluate the difference in battery temperature and airflow streamlines between the two solutions.

For the scenario studied in this model, the solutions obtained with the bidirectionally and unidirectionally coupled approaches are relatively close, while the unidirectionally coupled approach is much faster to solve.