

Jelly Roll

Introduction

A lithium battery cell is constructed as a sandwich of different layers (current collector metal foils, porous electrodes, separators), which is placed in an enclosure filled with electrolytes. The configuration of the sandwich depends on the type of enclosure (coin cell, prismatic, pouch, cylinder, and so on). Cylindrical lithium-ion batteries are manufactured by rolling the different battery layers into a cylindrical roll, which is then placed in a metal can. The resulting rolled spiral structure is commonly referred to as a "jelly roll."

The current collector foils are usually made of copper on the negative side and aluminum on the positive side, with thicknesses around tens of micrometers or less. To conduct the current to and from the jelly roll to the world exterior to the battery can, additional strips of metal are welded to the current collectors. These metal strips are called tabs. The simplest tabbing design, used in low-power batteries, places one tab on each side of the jelly roll (Ref. 1).

The interplay of the various dimensions of the layers and the tabs, in combination with the magnitude of the cell current, governs the temperature and current distribution in the battery cell.

This tutorial models the ohmic and activation losses, and the resulting temperature distribution, in a jelly roll for a pseudostationary case at a constant cell current.

Model Definition

Figure 1 shows the model geometry. The roll is 60 mm high, with a maximum outer spiral radius of 8.5 mm, and a minimum inner radius of 2 mm, including the cell tab. The tabs

extend 5 mm outside the jelly roll, the positive upward from the center of the spiral, the negative downward

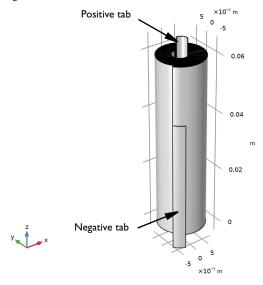


Figure 1: Model geometry.

Parametric curves, based on archimedal spiral functions are used to create the roll cross-sectional geometry, assuming a constant cell thickness. The following materials and thicknesses are used for the different layers, as indicated in Figure 2:

• Positive tab: aluminum, 100 mm thick, 4 mm wide

• Positive current collector: aluminum, 10 mm thick

• Positive electrode: NMC 111, 200 mm thick

• Separator: 30 mm thick

• Negative electrode: graphite, 200 mm thick

• Negative current collector: copper, 10 mm thick

• Negative tab: nickel, 100 mm thick, 4 mm wide

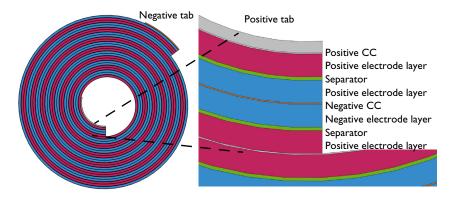


Figure 2: Cross section of the jelly roll.

The model in the tutorial uses a pseudostationary approach, only accounting for the ohmic voltage losses in the electronic conductors and the electrolyte and the activation overpotentials due to the charge transfer reactions in the electrodes. The current distribution is modeled using a **Secondary Current Distribution** interface.

This model is a simplification since it will be excluding any (tertiary) effects due to accumulation or depletion of lithium atoms in the electrodes or ions in the electrolyte. As soon as a current starts running through the battery, local concentration levels will change, which in turn impact the local electrolyte conductivity and equilibrium (half-cell) potentials of the electrodes, which will impact the current distribution over time. However, for a short period of time after turning on the current, a secondary current distribution model can accurately predict the voltage losses in the jelly roll.

In the current distribution model, a ground condition is used at the negative terminal, whereas a 1C total current condition is applied at the positive terminal.

The temperature distribution in the jelly roll is modeled using a **Heat Transfer** interface, applying the resulting heat sources from the current distribution model using an **Electrochemical Heating** multiphysics node. A convective cooling boundary condition on the outer area of the jelly roll is used, prescribing a cooling heat flux being proportional to the surface temperature and the exterior temperature (25°C). Heat being conducted through the electric terminals at the tab ends is ignored.

Figure 3 and Figure 4 show the simulated potential distribution in the negative and positive current collectors, respectively, for the jelly roll when subjected to a 1C discharge.

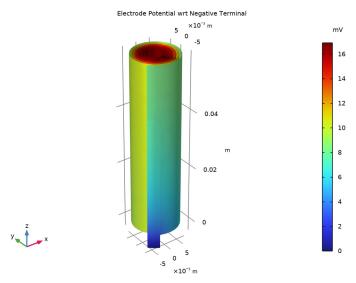


Figure 3: Potential in the negative current collector and tab.

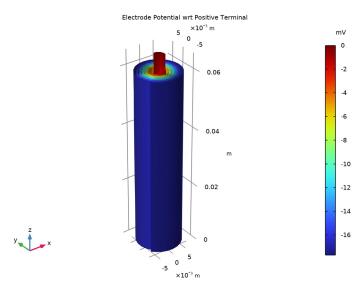


Figure 4: Potential in the positive current collector and tab.

Figure 5 shows a steep increase in temperature in the tabs close to the current terminals. This indicates that the Joule heating in the tabs results in significant local heating already for this fairly small battery at moderate currents. This is important since local temperature differences can result in the battery aging in an inhomogeneous way, which in turn may accelerate aging further.

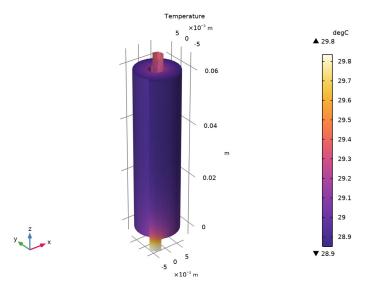


Figure 5: Temperature distribution.

Notes About the COMSOL Implementation

Assembly boundaries are placed in the middle of the separators, thereby allowing for sweeping the meshes in the through-plane direction.

Reference

1. X. Yao and M. Pecht, "Tab Design and Failures in Cylindrical Li-ion Batteries," *IEEE Access*, vol. 7, pp. 24082–24095, 2019.

Application Library path: Battery_Design_Module/Thermal_Management/jelly_roll

Modeling Instructions

This model is built in two parts. In the first part, a secondary current distribution model will be defined and solved. In the second part, heat transfer will included.

From the File menu, choose New.

NEW

In the New window, click Model Wizard.

MODEL WIZARD

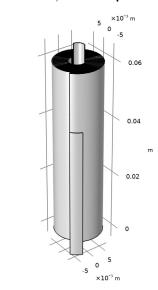
- I In the Model Wizard window, click 1 3D.
- 2 In the Select Physics tree, select Electrochemistry> Primary and Secondary Current Distribution>Secondary Current Distribution (cd).
- 3 Click Add.
- 4 Click Study.
- 5 In the Select Study tree, select General Studies>Stationary.
- 6 Click M Done.

GEOMETRY I

Insert a geometry sequence from a file.

- I 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 jelly_roll_geom_sequence.mph.
- 3 In the Geometry toolbar, click **Build All**.

4 In the Model Builder window, under Component I (compl) click Geometry I.



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GLOBAL DEFINITIONS

Geometry Parameters

By importing the sequence, some parameters were added to the model.

- I In the Model Builder window, under Global Definitions click Parameters I.
- 2 In the Settings window for Parameters, type Geometry Parameters in the Label text field.

Physics Parameters

Import additional parameters, needed to set up the physics, as follows:

- I In the Home toolbar, click Pi Parameters and choose Add>Parameters.
- 2 In the Settings window for Parameters, type Physics Parameters in the Label text field.
- 3 Locate the Parameters section. Click **Load from File**.
- **4** Browse to the model's Application Libraries folder and double-click the file jelly_roll_parameters.txt.

GEOMETRY I

In the Model Builder window, collapse the Component I (compl)>Geometry I node.

ADD MATERIAL

- I In the Home toolbar, click Radd Material to open the Add Material window.
- 2 Go to the Add Material window.
- 3 In the tree, select Built-in>Aluminum.
- 4 Right-click and choose Add to Component I (compl).
- 5 In the tree, select Built-in>Copper.
- 6 Right-click and choose Add to Component I (compl).
- 7 In the tree, select Battery>Electrodes>Graphite, LixC6 MCMB (Negative, Li-ion Battery).
- 8 Right-click and choose Add to Component I (compl).
- 9 In the tree, select Battery>Electrodes>NMC 111, LiNi0.33Mn0.33Co0.3302 (Positive, Liion Battery).
- 10 Right-click and choose Add to Component I (compl).
- II In the tree, select Battery>Electrolytes>LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery).
- 12 Right-click and choose Add to Component I (compl).
- 13 In the Home toolbar, click Radd Material to close the Add Material window.

MATERIALS

Aluminum (mat I)

- In the Settings window for Material, locate the Geometric Entity Selection section.
- 2 From the Selection list, choose Positive CC and Tab.

Copper (mat2)

- I 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.

Graphite, LixC6 MCMB (Negative, Li-ion Battery) (mat3)

- I In the Model Builder window, click Graphite, LixC6 MCMB (Negative, Liion Battery) (mat3).
- 2 In the Settings window for Material, locate the Geometric Entity Selection section.
- 3 From the Selection list, choose Negative Electrodes.

NMC 111, LiNi0.33Mn0.33Co0.33O2 (Positive, Li-ion Battery) (mat4)

I In the Model Builder window, click NMC III, LiNi0.33Mn0.33Co0.3302 (Positive, Liion Battery) (mat4).

- 2 In the Settings window for Material, locate the Geometric Entity Selection section.
- 3 From the Selection list, choose Positive Electrodes.

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

- I 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 Separators.

Nickel

The negative tab consists of nickel metal, which is not available in the material library. Add a blank material node for nickel for now. We will add the required parameters later.

- I In the Model Builder window, right-click Materials and choose Blank Material.
- 2 In the Settings window for Material, type Nickel in the Label text field.
- **3** Locate the **Geometric Entity Selection** section. From the **Selection** list, choose **Negative Tab**.

SECONDARY CURRENT DISTRIBUTION (CD)

Electrolyte I

Now start defining the current distribution model.

- I In the Model Builder window, under Component I (compl)>
 Secondary Current Distribution (cd) click Electrolyte I.
- 2 In the Settings window for Electrolyte, locate the Electrolyte section.
- **3** From the σ_1 list, choose **User defined**. In the associated text field, type sigmal eff.

Current Conductor I

- I In the Physics toolbar, click **Domains** and choose Current Conductor.
- 2 In the Settings window for Current Conductor, locate the Domain Selection section.
- 3 From the Selection list, choose CCs and Tabs.

The electrode node defines electronic conduction in the metal phase domains. The conductivity is taken from the Material nodes by default, so no additional settings are needed here.

Porous Electrode I

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

The porous electrode node defines both electronic and ionic conduction in the electrode and electrolyte phases, respectively. Since we use the same settings in the

positive and negative electrode materials in this tutorial, it suffices to use one single node.

- 2 In the Settings window for Porous Electrode, locate the Domain Selection section.
- **3** From the **Selection** list, choose **Electrodes**.
- **4** Locate the **Electrolyte Current Conduction** section. From the σ_l list, choose **User defined**. In the associated text field, type sigmal_eff.
- **5** From the **Effective conductivity correction** list, choose **No correction**.
- 6 Locate the Electrode Current Conduction section. From the σ_s list, choose User defined. In the associated text field, type sigmas eff.
- 7 From the Effective conductivity correction list, choose No correction.

Porous Electrode Reaction I

In this tutorial we are only interested in the voltage losses, not the resulting cell voltage. Therefore we use the default value of 0 V for the equilibrium potential in both electrodes. The resulting potential at the positive current terminal will thereby equal the total polarization of the cell.

- I In the Model Builder window, click Porous Electrode Reaction I.
- 2 In the Settings window for Porous Electrode Reaction, locate the Electrode Kinetics section.
- **3** From the Kinetics expression type list, choose Butler-Volmer.
- **4** In the i_0 text field, type i0.
- **5** Locate the **Active Specific Surface Area** section. In the $a_{\rm v}$ text field, type Av.

Electric Ground 1

- I 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 Current Terminal.

Electrode Current I

- I In the Physics toolbar, click **Boundaries** and choose **Electrode Current**.
- 2 In the Settings window for Electrode Current, locate the Boundary Selection section.
- 3 From the Selection list, choose Positive Current Terminal.
- **4** Locate the **Electrode Current** section. In the $I_{\rm s,total}$ text field, type I_1C.

MATERIALS

Nickel (mat6)

The Nickel material node is now with a small red cross, indicating a missing parameter value.

- I In the Model Builder window, under Component I (compl)>Materials click Nickel (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	1.4e7[S /m]	S/m	Basic

The small red cross should now have disappeared.

MESH I

Create a mesh sequence that sweeps the mesh in the radial direction of the spiral. The boundary faces located between the tabs and the current collector foils are meshed first. In this way, these faces will be used as source boundaries by the sweep operation, and the mid-separator boundaries will be used as destination boundaries. As prerequisite for sweeping the mesh is that, by the way the geometry sequence is set up, assembly boundaries are located in the middle of the separators. Using a geometry without an assembly would not allow for sweeping, since it would introduce faces on the destination boundaries that would not correspond to any faces on the source boundaries.

Size 1

- I In the Model Builder window, under Component I (compl) right-click Mesh I 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 Tabs.
- **5** Locate the **Element Size** section. Click the **Custom** button.
- 6 Locate the Element Size Parameters section.
- 7 Select the **Maximum element size** check box. In the associated text field, type H_tab_outside_jr/5.

Size

- I In the Model Builder window, click Size.
- 2 In the Settings window for Size, locate the Element Size section.
- **3** Click the **Custom** button.
- 4 Locate the Element Size Parameters section. In the Maximum element size text field, type H mesh.
- 5 In the Minimum element size text field, type D sep/2.

Free Quad I

- I In the Mesh toolbar, click A More Generators and choose Free Quad.
- 2 In the Settings window for Free Quad, locate the Boundary Selection section.
- 3 From the Selection list, choose Initial Mesh Faces.
- 4 Click Build Selected.

Swebt 1

In the Mesh toolbar, click A Swept.

Distribution 1

- I Right-click Swept I and choose Distribution.
- 2 In the Settings window for Distribution, locate the Domain Selection section.
- 3 From the Selection list, choose Separators.
- 4 Locate the Distribution section. In the Number of elements text field, type 2.

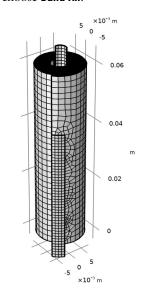
Distribution 2

- I In the Model Builder window, right-click Swept I and choose Distribution.
- 2 In the Settings window for Distribution, locate the Domain Selection section.
- 3 From the Selection list, choose Electrodes.

Distribution 3

- I Right-click **Swept I** and choose **Distribution**.
- 2 In the Settings window for Distribution, locate the Domain Selection section.
- 3 From the Selection list, choose CCs and Tabs.
- 4 Locate the Distribution section. In the Number of elements text field, type 2.

Swept I Right-click Swept I and choose Build All.





STUDY I

Now solve the current distribution model.

- I In the Model Builder window, click Study I.
- 2 In the Settings window for Study, locate the Study Settings section.
- 3 Clear the Generate default plots check box.
- 4 In the Home toolbar, click **Compute**.

RESULTS

Add plots for the potentials as follows:

Electrode Potential wrt Negative Terminal

- I In the Home toolbar, click Add Plot Group and choose 3D Plot Group.
- 2 In the Settings window for 3D Plot Group, type Electrode Potential wrt Negative Terminal in the Label text field.

Volume 1

I Right-click Electrode Potential wrt Negative Terminal and choose Volume.

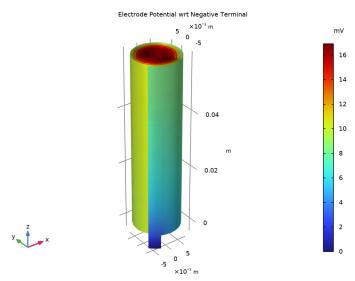
- 2 In the Settings window for Volume, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component I (compl)> Secondary Current Distribution>cd.phis - Electric potential - V.
- **3** Locate the **Expression** section. From the **Unit** list, choose **mV**.

Selection I

- I Right-click Volume I and choose Selection.
- 2 In the Settings window for Selection, locate the Selection section.
- 3 From the Selection list, choose Negative CC and Tab.

Electrode Potential wrt Negative Terminal

- I In the Model Builder window, under Results click **Electrode Potential wrt Negative Terminal.**
- 2 In the Settings window for 3D Plot Group, click to expand the Title section.
- 3 From the Title type list, choose Label.
- **4** Locate the **Color Legend** section. Select the **Show units** check box.
- 5 Locate the Plot Settings section. Clear the Plot dataset edges check box.
- 6 In the Electrode Potential wrt Negative Terminal toolbar, click **Plot**.



7 Right-click Results>Electrode Potential wrt Negative Terminal and choose Duplicate.

Electrode Potential wrt Positive Terminal

- I In the Model Builder window, under Results click Electrode Potential wrt Negative Terminal I.
- 2 In the Settings window for 3D Plot Group, type Electrode Potential wrt Positive Terminal in the Label text field.

Volume 1

- I In the Model Builder window, expand the Electrode Potential wrt Positive Terminal node, then click Volume I.
- 2 In the Settings window for Volume, click Insert Expression (Ctrl+Space) in the upper-right corner of the Expression section. From the menu, choose Component I (compl)> Secondary Current Distribution>cd.phis0_ecl Electric potential on boundary V.
- 3 Locate the Expression section. In the Expression text field, type cd.phis-cd.phis0_ec1.
- 4 From the Unit list, choose mV.

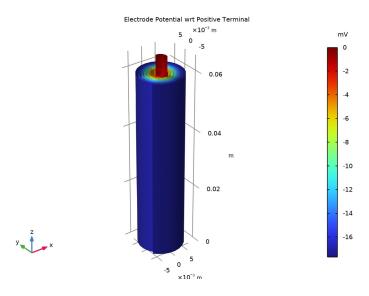
Selection I

- I In the Model Builder window, expand the Volume I node, then click Selection I.
- 2 In the Settings window for Selection, locate the Selection section.
- 3 From the Selection list, choose Positive CC and Tab.

Electrode Potential wrt Positive Terminal

I In the Model Builder window, under Results click
Electrode Potential wrt Positive Terminal.

2 In the Electrode Potential wrt Positive Terminal toolbar, click Plot.



COMPONENT I (COMPI)

Now we move over to the second part of this tutorial, in which we will include heat transfer.

ADD PHYSICS

- I In the Home toolbar, click Add Physics to open the Add Physics window.
- 2 Go to the Add Physics window.
- 3 In the tree, select Heat Transfer>Heat Transfer in Solids (ht).
- 4 Click Add to Component I in the window toolbar.
- 5 In the Home toolbar, click Add Physics to close the Add Physics window.

HEAT TRANSFER IN SOLIDS (HT)

Solid 1

The default **Solid** node will define heat transfer in all domains. The thermal conductivity is taken from the materials nodes by default. Since we will defining a stationary problem, the density and the heat capacity are not needed.

I In the Model Builder window, under Component I (compl)>Heat Transfer in Solids (ht) click Solid 1.

- 2 In the Settings window for Solid, locate the Thermodynamics, Solid section.
- **3** From the ρ list, choose User defined. From the C_p list, choose User defined.

Initial Values 1

- I In the Model Builder window, 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 ext.

Heat Flux I

Add a convective heat flux to the outer jelly roll envelope. This condition corresponds to an air-cooled surface using a fairly low air flow velocity.

- I In the Physics toolbar, click **Boundaries** and choose **Heat Flux**.
- 2 In the Settings window for Heat Flux, locate the Boundary Selection section.
- 3 From the Selection list, choose Cooling Boundaries.
- 4 Locate the Heat Flux section. From the Flux type list, choose Convective heat flux.
- **5** In the *h* text field, type hT.
- **6** In the $T_{\rm ext}$ text field, type T_ext.

MULTIPHYSICS

Add an electrochemical heating node. This node will apply the heat sources calculated by the current distribution model to the heat transfer model.

Electrochemical Heating I (ech I)

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

MATERIALS

We need also to add missing parameters for the thermal conductivity to some of the material nodes.

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

- I In the Model Builder window, under Component I (compl)>Materials 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	, ,	0.35[W/ (m*K)]	W/(m·K)	Basic

Nickel (mat6)

- I In the Model Builder window, click Nickel (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
Thermal conductivity	k_iso ; kii = k_iso, kij = 0	100[W/ (m*K)]	W/(m·K)	Basic

HEAT TRANSFER IN SOLIDS (HT)

Lower the discretization order of heat transfer to use linear elements. This will shorten the computation time and lower the memory requirements.

- I In the Model Builder window, under Component I (compl) click Heat Transfer in Solids (ht).
- 2 In the Settings window for Heat Transfer in Solids, click to expand the Discretization section.
- 3 From the Temperature list, choose Linear.

Alter the study so that you first solve for the current distribution, and then heat transfer model.

STUDY I

Step 1: Stationary

- I In the Model Builder window, under Study I click Step I: Stationary.
- 2 In the Settings window for Stationary, locate the Physics and Variables Selection section.

3 In the table, enter the following settings:

Physics interface	Solve for	Equation form
Secondary Current Distribution (cd)	V	Automatic (Stationary)
Heat Transfer in Solids (ht)		Automatic (Stationary)

Step 2: Stationary 2

- I In the Study toolbar, click Study Steps and choose Stationary>Stationary.
- 2 In the Settings window for Stationary, locate the Physics and Variables Selection section.
- **3** In the table, enter the following settings:

Physics interface	Solve for	Equation form
Secondary Current Distribution (cd)		Automatic (Stationary)
Heat Transfer in Solids (ht)	V	Automatic (Stationary)

Solution I (soll)

- I In the Model Builder window, right-click Solver Configurations and choose Reset Solver to Default.
- 2 Expand the Solution I (soll) node.
 Inspect the solver sequence. The sequence should now consist of two stationary solvers.
- 3 In the Model Builder window, expand the Study I>Solver Configurations> Solution I (soll)>Stationary Solver 2 node.
- 4 Right-click Study I and choose Compute.

RESULTS

Create a temperature plot as follows:

Temperature

- I In the Home toolbar, click Add Plot Group and choose 3D Plot Group.
- 2 In the Settings window for 3D Plot Group, type Temperature in the Label text field.

Volume 1

- I Right-click Temperature and choose Volume.
- 2 In the Settings window for Volume, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component I (compl)> Heat Transfer in Solids>Temperature>T Temperature K.

- 3 Locate the Expression section. From the Unit list, choose degC.
- 4 Locate the Coloring and Style section. Click | Change Color Table.
- 5 In the Color Table dialog box, select Thermal>HeatCameraLight in the tree.
- 6 Click OK.

Temperature

- I In the Model Builder window, click Temperature.
- 2 In the Settings window for 3D Plot Group, locate the Title section.
- 3 From the Title type list, choose Label.
- 4 Locate the Plot Settings section. Clear the Plot dataset edges check box.
- 5 Locate the Color Legend section. Select the Show maximum and minimum values check box.
- 6 Select the **Show units** check box.
- 7 In the Temperature toolbar, click **Plot**.

