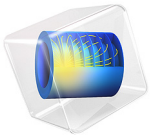


Thermal Modeling of a Cylindrical Lithium-Ion Battery in 2D

Introduction

Thermal management is crucial for safety and for ensuring long lifetimes of batteries. High temperatures typically shorten the battery lifetime by increasing the rate of the degrading processes, and therefore active cooling may be needed for high power applications. Another aspect of thermal management is that large temperature gradients within a single battery, or battery pack, need to be avoided since they may lead to non-uniform current densities and non-uniform aging phenomena.

The varying length scales and complex geometries of a Li-ion battery requires some consideration. The individual layers forming the battery cells are typically of the scale of tens of micrometers in the normal direction to the layers, but up to tens of centimeters in the sheet direction, and are usually wound into multilayer geometries. When it comes to the actual battery or battery pack, the geometries may be in the scale of centimeters up to meters (for the case of an electric vehicle), and can consist of hundreds of individual cells. Resolving these geometries with a full three-dimensional model of the battery chemistry is computationally costly.

However, since the heat conductivity of the components of a lithium-ion battery is quite high in relation to the heat generated, one can in many cases assume the battery to have a fairly uniform temperature profile. Furthermore, if the battery chemistry is not heavily affected by small temperature changes, little detail is lost by describing the battery chemistry using a lumped model, based on the average temperature of the battery.

This example simulates an air-cooled cylindrical 18650 lithium-ion battery during a charge-discharge cycle, followed by a relaxing period. A lumped battery model is used to model the battery cell chemistry, and a two-dimensional axisymmetrical model is used to model the temperature in the battery. The two models are coupled by the generated heat source and the average temperature using the Electrochemical Heating multiphysics coupling node.

Model Definition

CELL MODEL

The cell model is created using the Lumped Battery interface. The interface requires inputs such as the battery capacity and initial state-of-charge, and consists of lumped parameters that represent the ohmic, activation and concentration overpotential contributions. A detailed description on how to optimize the parameters of the lumped model against experimental data can be found in the Application Libraries example Parameter Estimation of a Time-Dependent Lumped Battery Model.

The lumped model can either solved in a *global* version, where the battery variables are defined globally, or in a *local* version where the variables are solved for locally in the same spatial dimension as the heat transfer physics interface. In this model, the Lumped Battery interface uses the *global* model of coupling to the Heat Transfer in Solids interface. The *global* model requires an average (global) value of temperature from the Heat Transfer interface and similarly provides an average value of the generated heat source in the active material domain to the Heat Transfer interface. On the other hand, the *local* model requires the local value of temperature in the active material domain from the Heat Transfer interface and provides the local value of the generated heat source to the Heat Transfer interface. The *local* model can be used when there is a large variation in temperature across the active battery material, and it becomes essential to consider local values of the generated heat source in the thermal model.

The Electrochemical Heating multiphysics coupling node is used to couple the temperature and the generated heat source between the Lumped Battery and Heat Transfer in Solids interfaces.

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 2. (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 20%.

THERMAL MODEL

The thermal model is in 2D with axial symmetry, using the Heat Transfer in Solids interface. The reason for using axial symmetry is that, for a spirally wound battery of this type, the heat conduction in the spiral direction can be neglected (Ref. 2). Furthermore, rather than modeling the heat conduction in each layer of the wound sheets in the radial direction (for example, in each positive electrode layer, each separator layer, and so on), the wound sheets are modeled as one active battery material domain. These approximations have been shown to be reasonable for spiral wound battery cells cooled by natural convection (Ref. 2).

The geometry (9 mm radius, 65 mm high, see Figure 1) consists of three domains:

- Battery canister (steel, 0.25 mm thick)
- Active battery material domain (wound sheets of cell material)

- Mandrel (isolator around which the battery cell sheets are wound, 2 mm radius)

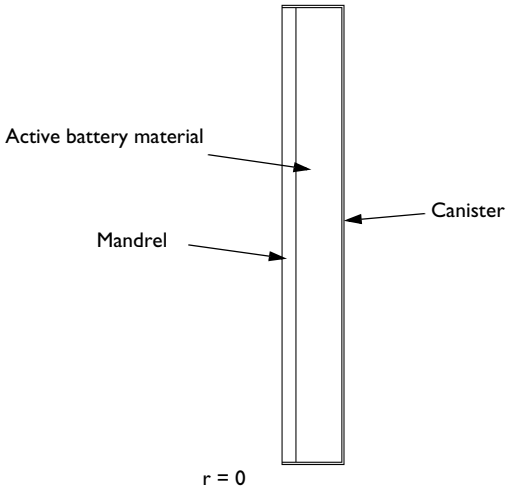


Figure 1: Geometry of the thermal model

The active battery material is assumed to consist of one or several battery cells wound spirally into a cylinder. As an effect of this, the thermal conductivities are anisotropic in the thermal model, with a higher thermal conductivity along the battery sheets, the cylinder length direction, than in the normal direction to the sheets, the radial direction (see Ref. 1).

In the radial direction the thermal conductivity, $k_{T,r}$, is calculated from the formula

$$k_{T,r} = \frac{\sum L_i}{\sum L_i / k_{T,i}}$$

where L_i are the thicknesses of the different layers of the cell, and $k_{T,i}$ the thermal conductivities of the materials constituting these layers.

The thermal conductivity in the cylinder length direction, $k_{T,\text{ang}}$, is calculated according to

$$k_{T,\text{ang}} = \frac{\sum L_i k_{T,i}}{\sum L_i}$$

The density, ρ_{batt}, and heat capacity, $C_{p,\text{batt}}$, for the active battery material are calculated similarly according to

$$\rho_{\text{batt}} = \frac{\sum L_i \rho_i}{\sum L_i}$$

$$C_{p,\,\text{batt}} = \frac{\sum L_i C_{p,\,i}}{\sum L_i}$$

The heat source generated in the active battery material domain is specified using the Electrochemical Heating multiphysics coupling node.

On the battery canister surface, a heat flux boundary condition is specified using a heat transfer coefficient of $h = 20$ W/(m^2·K) and an external temperature of 298.15 K. This would typically correspond to air cooling by low velocity forced convection.

The initial temperature of the battery is set to 298.15 K.

Figure 2 shows the cell potential and the load cycle current.

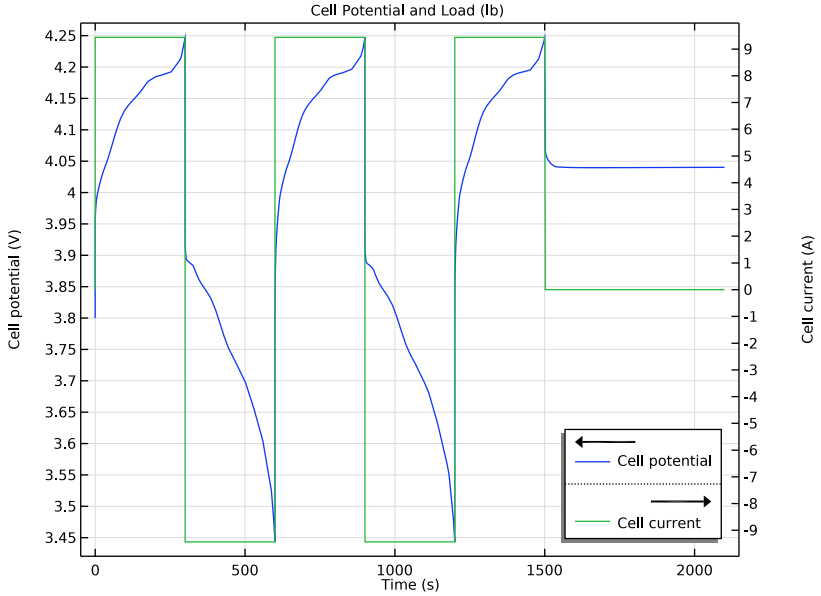


Figure 2: Cell potential and current load.

Figure 3 shows the maximum, minimum and average temperatures of the battery during the simulation. The temperature differences between the minimum and maximum never exceed 3 K. Also, the difference in heating rate between charge and discharge is due to the entropy effects (reversible heating).

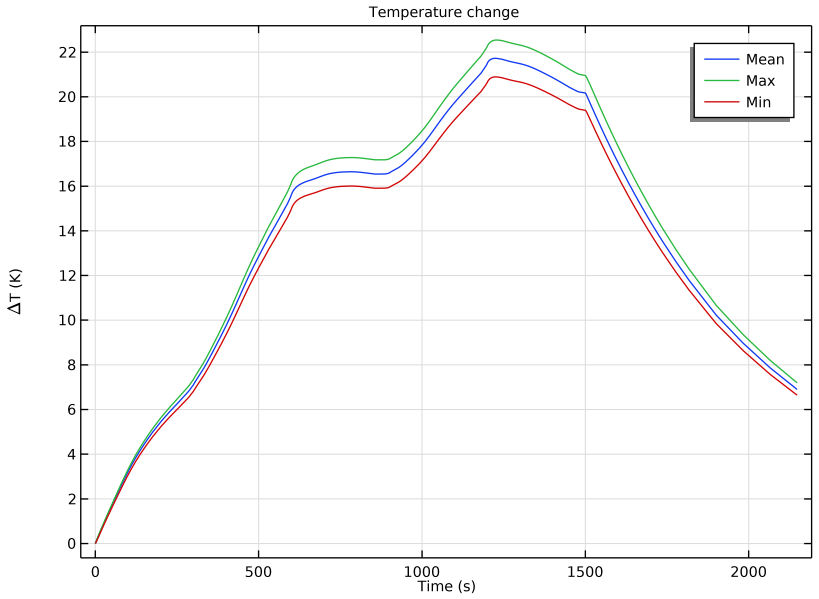


Figure 3: Mean, maximum, and minimum temperature.

Returning to Figure 2 it is also seen that the cell potential of the different cycles is not largely affected by the small temperature changes in Figure 3. Note that the battery model currently includes temperature dependence of the open circuit voltage. Additionally, it could include temperature dependence of the lumped parameters.

Figure 4 shows the temperature in the battery cylinder at 1500 s. The temperature maximum is located in the active battery material in the center of the battery.

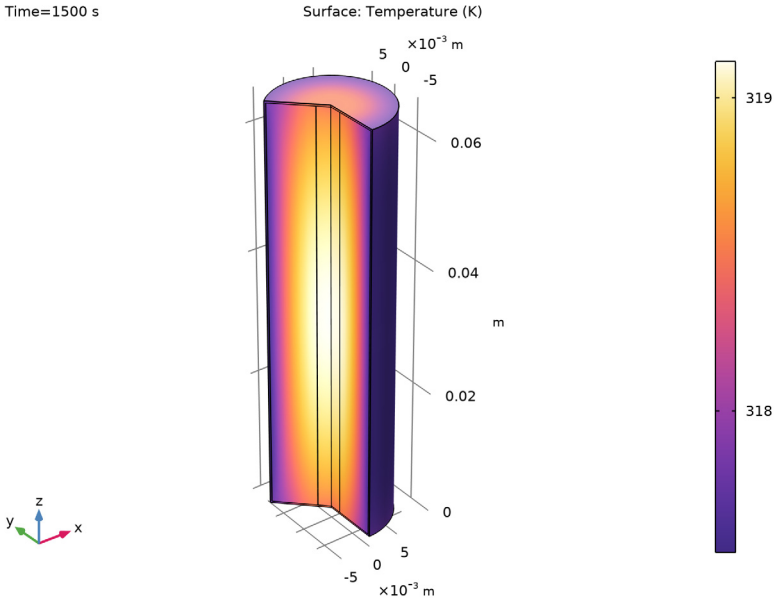


Figure 4: Temperature distribution in the battery at t=1500 s.

References

1. S.-C. Chen, Y.-Y. Wang, and C.-C. Wan, "Thermal Analysis of Spirally Wound Lithium Batteries", *J. Electrochem. Soc.*, vol. 153, no. 4, pp. A637–A648, 2006.

2. P.M. Gomadam, R.E. White, and J.W. Weidner, "Modeling Heat Conduction in Spiral Geometries", *J. Electrochem. Soc.*, vol. 150, no. 10, pp. A1339–A1345, 2003.

Application Library path: `Battery_Design_Module/Thermal_Management/li_battery_thermal_2d_axi`

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 Axisymmetric**.

2 In the **Select Physics** tree, select **Electrochemistry>Batteries>Lumped Battery (lb)**.

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 **General Studies>Time Dependent**.

8 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.

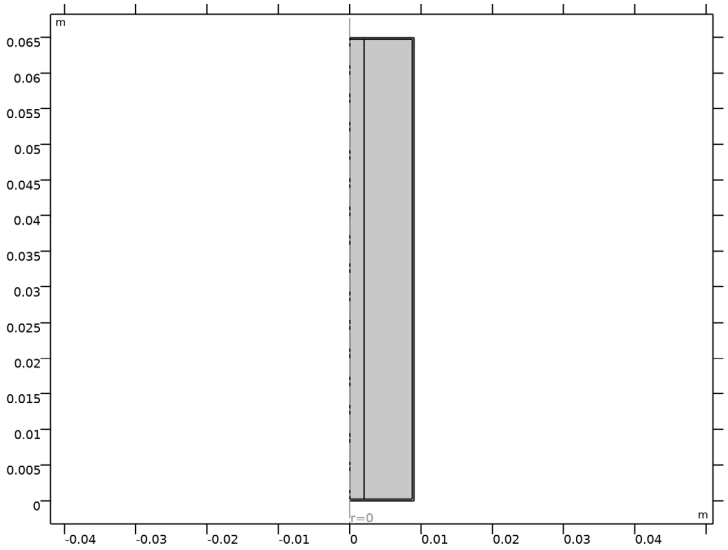
1 In the **Geometry** toolbar, click **Insert Sequence** and choose **Insert Sequence**.

2 Browse to the model's Application Libraries folder and double-click the file `li_battery_thermal_2d_axi_geom_sequence.mph`.

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

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

The geometry should be as shown below:



GLOBAL DEFINITIONS

Load parameters from a text file. Note that the node already contains parameters that were used for building the geometry.

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 `li_battery_thermal_2d_axi_parameters.txt`.

Waveform 1 (wv1)

Create a waveform function to define the applied current.

1 In the **Home** toolbar, click **Functions** and choose **Global>Waveform**.

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

3 From the **Type** list, choose **Square**.

4 In the **Period** text field, type `cycle_time`.

DEFINITIONS

Variables 1

1 In the **Home** toolbar, click **Variables** and choose **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
Iapp	lb.I_1C*7.5*(wv1(t))*(t<1500)	A	Applied current

Mean Temperature

Create probes for the mean, max, and min temperature changes in the thermal model.

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

2 In the **Settings** window for **Domain Probe**, type `Mean Temperature` in the **Label** text field.

3 In the **Variable name** text field, type `MeanT`.

4 Locate the **Source Selection** section. From the **Selection** list, choose **Active Battery Material**.

5 Locate the **Expression** section. In the **Expression** text field, type `T-T_init`.

6 Click to expand the **Table and Window Settings** section. Click **Add Plot Window**.

Max Temperature

1 Right-click **Mean Temperature** and choose **Duplicate**.

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

3 In the **Variable name** text field, type `maxT`.

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

Min Temperature

1 Right-click **Max Temperature** and choose **Duplicate**.

2 In the **Settings** window for **Domain Probe**, type `Min Temperature` in the **Label** text field.

3 In the **Variable name** text field, type `minT`.

4 Locate the **Probe Type** section. From the **Type** list, choose **Minimum**.

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>Steel AISI 4340**.

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

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

MATERIALS

Steel AISI 4340 (mat1)

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

2 From the **Selection** list, choose **Battery Can**.

LUMPED BATTERY (LB)

You will now start defining the lumped battery model.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Lumped Battery (lb)**.

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

3 From the **Selection** list, choose **Active Battery Material**.

4 Locate the **Operation Mode** section. In the I_{app} text field, type `Iapp`.

5 Locate the **Battery Settings** section. In the $Q_{\text{cell},0}$ text field, type `Q_batt`.

6 In the $\text{SOC}_{\text{cell},0}$ text field, type `SOC_init`.

Cell Equilibrium Potential 1

Load the open circuit voltage data at reference temperature and the temperature derivative of open circuit voltage data from text files into the tables below.

The temperature derivative of open circuit voltage data is used to calculate the temperature dependence of the open circuit voltage. Also, this data is used in the calculation of the reversible (entropic) contribution and heat of mixing contribution to the total heat source.

1 In the **Model Builder** window, under **Component 1 (comp1)>Lumped Battery (lb)** click **Cell Equilibrium Potential 1**.

2 In the **Settings** window for **Cell Equilibrium Potential**, locate the **Open Circuit Voltage** section.

3 Click **Clear Table**.

Note that it is important to clear the tables before loading data from the text files.

4 Click **Load from File**.

5 Browse to the model's Application Libraries folder and double-click the file `li_battery_thermal_2d_axi_E_OCP_data.txt`.

6 Click **Clear Table**.

7 Click **Load from File**.

8 Browse to the model's Application Libraries folder and double-click the file `li_battery_thermal_2d_axi_dEdT_data.txt`.

Voltage Losses 1

Set up the lumped parameters of the battery model.

1 In the **Model Builder** window, click **Voltage Losses 1**.

2 In the **Settings** window for **Voltage Losses**, locate the **Ohmic Overpotential** section.

3 In the $\eta_{IR,1C}$ text field, type `eta_ohmic1C`.

4 Locate the **Activation Overpotential** section. In the J_0 text field, type `J0`.

5 Locate the **Concentration Overpotential** section. Select the **Include concentration overpotential** check box.

6 In the τ text field, type `tau`.

HEAT TRANSFER IN SOLIDS (HT)

Set up the heat transfer model that consists of three solid domains representing the battery can, active battery material and mandrel domains, respectively.

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

Solid 2

1 In the **Physics** toolbar, click **Domains** 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 **Heat Conduction, Solid** section. From the k list, choose **User defined**. From the list, choose **Diagonal**.

5 In the k table, enter the following settings:

`kT_batt_r`	`0`
`0`	`kT_batt_ang`

6 Locate the **Thermodynamics, Solid** section. From the ρ list, choose **User defined**. In the associated text field, type `rho_batt`.

7 From the C_p list, choose **User defined**. In the associated text field, type `Cp_batt`.

Solid 3

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

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

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

4 Locate the **Heat Conduction, Solid** section. From the k list, choose **User defined**. In the associated text field, type `kT_sep`.

5 Locate the **Thermodynamics, Solid** section. From the ρ list, choose **User defined**. In the associated text field, type `rho_sep`.

6 From the C_p list, choose **User defined**. In the associated text field, type `Cp_sep`.

Heat Flux 1

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

2 Select Boundaries 2, 7, and 12 only.

3 In the **Settings** window for **Heat Flux**, locate the **Heat Flux** section.

4 From the **Flux type** list, choose **Convective heat flux**.

5 In the h text field, type `20`.

6 In the T_{ext} text field, type `T_init`.

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 `T_init`.

MULTIPHYSICS

Set up the coupling between the battery interface and the heat transfer interface using the **Electrochemical Heating** multiphysics coupling node.

Electrochemical Heating 1 (ech1)

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

MESH 1

Mapped 1

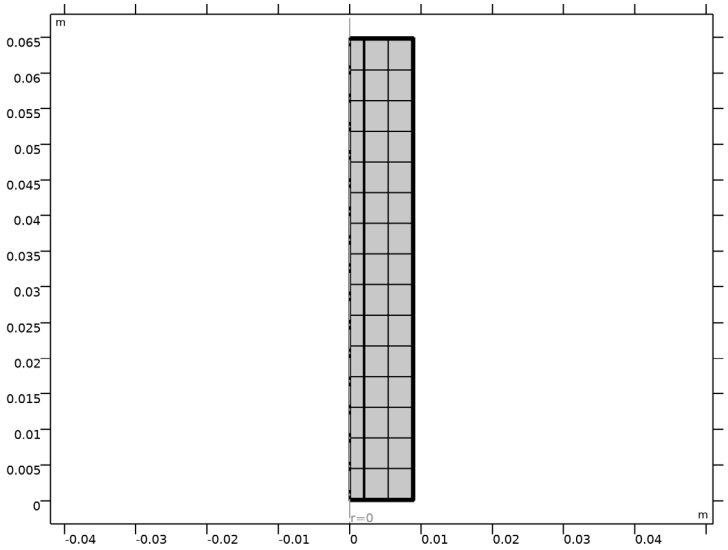
1 In the **Mesh** toolbar, click **Mapped**.

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

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

4 In the **Model Builder** window, right-click **Mesh 1** and choose **Build All**.

The mesh should be as shown below:



STUDY 1

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 1** click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

3 In the **Output times** text field, type `0 2100`.

4 From the **Tolerance** list, choose **User controlled**.

5 In the **Relative tolerance** text field, type `1e-3`.

Solution 1 (sol1)

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

Store the actual steps taken by the solver to make sure to capture any sudden steep voltage changes.

2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node, then click **Time-Dependent Solver 1**.

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

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

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

6 Click on the Probe Plot 1 tab to place the probe plot in focus while solving.

RESULTS

When the solver has finished you have four default plots in addition to the probe plot.

Cell Potential and Load (lb)

First, modify the Cell potential and load plot to show only the cell potential and load cycle current. To achieve this, disable the global plot that plots the cell open circuit voltage. Compare with Figure 2.

Global 2

1 In the **Model Builder** window, expand the **Cell Potential and Load (lb)** node.

2 Right-click **Global 2** and choose **Disable**.

Cell Potential and Load (lb)

1 In the **Model Builder** window, click **Cell Potential and Load (lb)**.

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

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

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

5 In the **Cell Potential and Load (lb)** toolbar, click **Plot**.

Temperature, 3D (ht)

This plot shows the temperature inside the battery at the end of the simulation interval. Change the time to 1500 s. Compare the resulting plot with that shown in Figure 4.

1 In the **Model Builder** window, click **Temperature, 3D (ht)**.

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

3 From the **Time (s)** list, choose **Interpolation**.

4 In the **Time** text field, type `1500`.

5 In the **Temperature, 3D (ht)** toolbar, click **Plot**.

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

Temperature vs. Time

Finally, modify this probe plot to reproduce the plot in Figure 3.

1 In the **Model Builder** window, under **Results** click **Probe Plot Group 5**.

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

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

4 In the **Title** text area, type `Temperature change`.

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

6 In the associated text field, type `\DELTA T (K)`.

Probe Table Graph 1

1 In the **Model Builder** window, expand the **Temperature vs. Time** node, then click **Probe Table Graph 1**.

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

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

4 In the table, enter the following settings:

Legends
Mean
Max
Min

Temperature vs. Time

1 In the **Model Builder** window, click **Temperature vs. Time**.

2 In the **Temperature vs. Time** toolbar, click **Plot**.

Appendix — Geometry Modeling Instructions

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

NEW

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

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 `li_battery_thermal_2d_axi_geom_sequence_parameters.txt`.

ADD COMPONENT

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

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_batt`.

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

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

Layer name	Thickness (m)
Layer 1	d_can
Layer 2	h_batt-d_can*2

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 `r_batt-d_can`.

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

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

Layer name	Thickness (m)
Layer 1	r_mandrel

6 Select the **Layers to the left** check box.

7 Clear the **Layers on bottom** check box.

8 Click **Build All Objects**.

Mesh Control Edges 1 (mce1)

1 In the **Geometry** toolbar, click **Virtual Operations** and choose **Mesh Control Edges**.

2 In the **Settings** window for **Mesh Control Edges**, locate the **Input** section.

3 Click **Paste Selection**.

4 In the **Paste Selection** dialog box, type `8, 12, 15, 18-20` in the **Selection** text field.

5 Click **OK**.

Battery Can

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

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

3 On the object **mce1**, select Domain 1 only.

Active Battery Material

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

2 In the **Settings** window for **Explicit Selection**, type `Active Battery Material` in the **Label** text field.

3 On the object **mce1**, select Domain 3 only.

Mandrel

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

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

3 On the object **mce1**, select Domain 2 only.