

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

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Introduction

This example simulates an air-cooled cylindrical 18650 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.

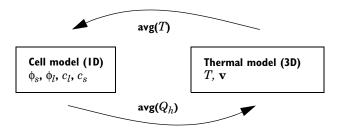


Figure 1: Coupling between the cell and thermal model using the average values for the temperature and generated heat.

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_xC₆ MCMB, 55 μm)
- Separator (30 µm)
- Positive porous electrode $(Li_vMn_2O_4, 55 \ \mu m)$

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)

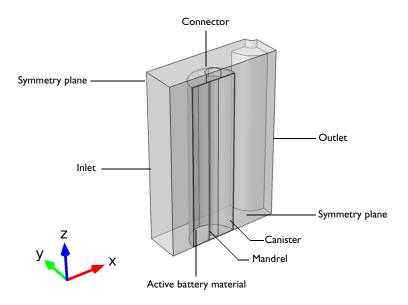


Figure 2: Geometry of the thermal model

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.

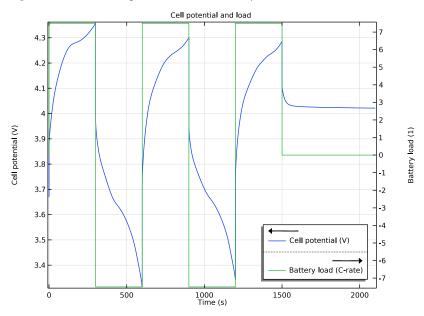


Figure 3: Cell potential and current load.

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).

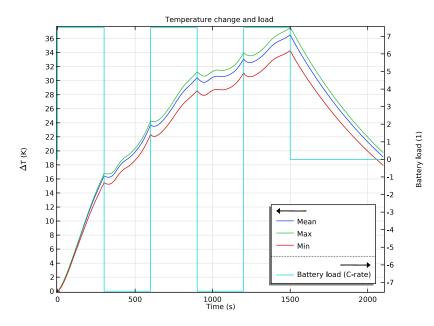


Figure 4: Minimum, mean, and maximum temperature.

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

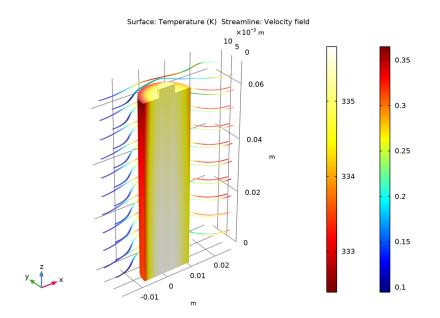


Figure 5: Temperature and flow at t=1500 s.

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.

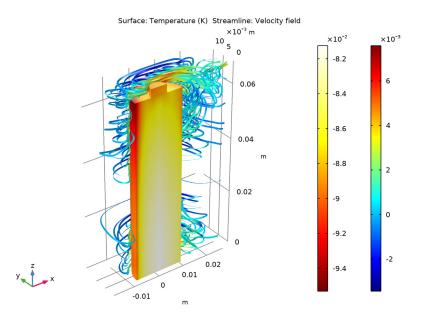


Figure 6: Differences in battery temperature and fluid flow streamlines between the coupled and one-way solutions after 2100 s.

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

ROOT

I From the File menu, choose Open.

2 Browse to the model's Application Libraries folder and double-click the file li_battery_1d_for_thermal_models.mph.

ADD COMPONENT

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

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 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 🖄 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 1 (nitf1)

In the Physics toolbar, click An Multiphysics 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

Name	Expression	Value	Description
V_in	0.1[m/s]	0.1 m/s	Inlet velocity
t	0	0	Time parameter in initialization study step

GEOMETRY 2

Cylinder I (cyl1)

- 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 틤 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 틤 Build Selected.

Union I (uniI)

- I In the Geometry toolbar, click P 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 (blk1)

- 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 틤 Build Selected.

Intersection 1 (int1)

- I In the Geometry toolbar, click i 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 틤 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 틤 Build 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 问 **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 틤 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 틤 Build Selected.

Difference I (dif1)

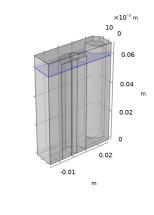
- I In the Geometry toolbar, click i Booleans and Partitions and choose Difference.
- 2 Select the objects **blk2**, **blk3**, and **int1** only.
- 3 In the Settings window for Difference, locate the Difference section.
- 4 Find the Objects to subtract subsection. Select the 💷 Activate Selection toggle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

Mesh Control Faces 1 (mcf1)

- I In the Geometry toolbar, click 🏷 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 \leftarrow **Zoom Extents** button in the **Graphics** toolbar.



y z x

DEFINITIONS (COMP2)

Flow Compartment

- I In the Definitions toolbar, click 堶 Explicit.
- 2 Right-click Explicit 4 and choose Rename.
- 3 In the Rename Explicit dialog box, type Flow Compartment in the New label text field.
- 4 Click OK.
- **5** Select Domain 1 only.

Active Battery Material

- I In the Definitions toolbar, click 堶 Explicit.
- 2 In the Model Builder window, right-click Explicit 5 and choose Rename.
- **3** In the **Rename Explicit** dialog box, type Active Battery Material in the **New label** text field.

4 Click OK.

5 Select Domain 2 only.

Battery Connector

- I In the Definitions toolbar, click 🐂 Explicit.
- 2 Right-click **Explicit 6** and choose **Rename**.

- 3 In the Rename Explicit dialog box, type Battery Connector in the New label text field.
- 4 Click OK.
- **5** Select Domain 3 only.

Mandrel

- I In the Definitions toolbar, click 🗞 Explicit.
- 2 In the Model Builder window, right-click Explicit 7 and choose Rename.
- 3 In the Rename Explicit dialog box, type Mandrel in the New label text field.
- 4 Click OK.
- **5** Select Domain 4 only.

Inlet

- I In the **Definitions** toolbar, click **here Explicit**.
- 2 Right-click Explicit 8 and choose Rename.
- 3 In the Rename Explicit dialog box, type Inlet in the New label text field.
- 4 Click OK.
- 5 In the Settings window for Explicit, locate the Input Entities section.
- 6 From the Geometric entity level list, choose Boundary.
- 7 Select Boundary 1 only.

Outlet

- I In the **Definitions** toolbar, click **herefore Explicit**.
- 2 In the Model Builder window, right-click Explicit 9 and choose Rename.
- 3 In the Rename Explicit dialog box, type Outlet in the New label text field.
- 4 Click OK.
- 5 In the Settings window for Explicit, locate the Input Entities section.
- 6 From the Geometric entity level list, choose Boundary.
- **7** Select Boundary 26 only.

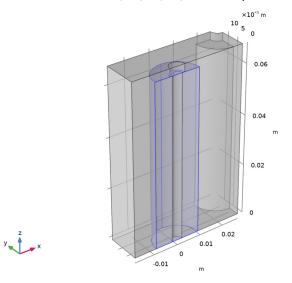
Symmetry planes

- I In the **Definitions** toolbar, click **here Explicit**.
- 2 Right-click Explicit 10 and choose Rename.
- 3 In the Rename Explicit dialog box, type Symmetry planes in the New label text field.
- 4 Click OK.
- 5 In the Settings window for Explicit, locate the Input Entities section.

- 6 From the Geometric entity level list, choose Boundary.
- 7 Select Boundaries 2, 5, and 22 only.

Can

- I In the **Definitions** toolbar, click **here Explicit**.
- 2 In the Model Builder window, right-click Explicit 11 and choose Rename.
- 3 In the Rename Explicit dialog box, type Can in the New label text field.
- 4 Click OK.
- 5 In the Settings window for Explicit, locate the Input Entities section.
- 6 From the Geometric entity level list, choose Boundary.
- 7 Select Boundaries 7–9, 12, 16, 17, and 20 only.



Average I (aveop 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.

DEFINITIONS (COMPI)

Now go to Component 1 (the 1D battery model) and define a model input for the average temperature from the 3D thermal model. Use nojac() to improve the time-dependent solver convergence.

Model Input 1

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

Average 2 (aveop2)

I In the Definitions toolbar, click 🖉 Nonlocal 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/m ³	Average heat source from 1d battery model
r	<pre>sqrt(x^2+y^2)</pre>	m	Radius

DEFINITIONS (COMPI)

Point Probe Expression 1 (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 1 (dom 1)

- 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 🙀 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.
- **IO** 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 \sum_{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 ρ 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 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 I

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

Temperature 1

- 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_in.

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_{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.

Swept I

- I In the Mesh toolbar, click 🆓 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 \land 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.

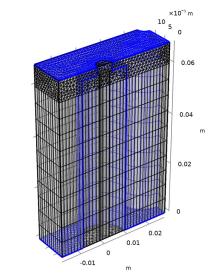
Boundary Layers 1

- 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 Boundary Layer Properties section.
- 4 In the Number of boundary layers text field, type 2.
- 5 From the Thickness of first layer list, choose Manual.
- 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 $\stackrel{\text{res}}{\longrightarrow}$ 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 $\stackrel{\text{res}}{\longrightarrow}$ 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).

Current Distribution Initialization

- I In the Study toolbar, click Current Distribution Initialization.
- 2 In the Settings window for Current Distribution Initialization, locate the Physics and Variables Selection section.
- 3 In the table, clear the Solve for check boxes for Laminar Flow (spf) and Heat Transfer in Solids and Fluids (ht).
- 4 In the table, clear the Solve for check box for Nonisothermal Flow I (nitfl).

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 timestepping 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 1 (soll)

By making a few further changes to the time-dependent solver, we can improve convergence. The strict timestepping 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 **The 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 Select the Initial step check box.
- 5 From the Steps taken by solver list, choose Strict.
- 6 Click to expand the Advanced section. Locate the Time Stepping section. Find the Algebraic variable settings subsection. From the Consistent initialization list, choose Off.
- 7 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.
- 8 In the Settings window for Segregated Step, click to expand the Method and Termination section.
- 9 From the Nonlinear method list, choose Automatic (Newton).
- **IO** Right-click **Battery current distribution** and choose **Move Up**.
- II In the Model Builder window, click Study I.
- 12 In the Settings window for Study, locate the Study Settings section.
- **I3** Clear the **Generate default plots** check box.
- **I4** 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 I.
- 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.

- 7 In the associated text field, type Cell potential (V).
- 8 Select the Secondary y-axis label check box.
- **9** In the associated text field, type Battery load (1).
- 10 Locate the Legend section. From the Position list, choose Lower right.

Cell Potential

- I In the Model Builder window, right-click Probe Table Graph I and choose Rename.
- 2 In the Rename Table Graph dialog box, type Cell Potential in the New label text field.
- 3 Click OK.
- 4 In the Settings window for Table Graph, click to expand the Legends section.
- 5 From the Legends list, choose Manual.
- **6** In the table, enter the following settings:

Legends

Cell potential (V)

Battery load (C-rate)

- I Right-click Cell Potential and choose Duplicate.
- 2 In the Settings window for Table Graph, locate the Data section.
- 3 In the Columns list, select i_app/i_IC (I).
- 4 Locate the Legends section. In the table, enter the following settings:

Legends

Battery load (C-rate)

- 5 Locate the y-Axis section. Select the Plot on secondary y-axis check box.
- 6 In the Probe Plot Group I toolbar, click 🗿 Plot.
- 7 Right-click Cell Potential I and choose Rename.
- 8 In the **Rename Table Graph** dialog box, type Battery load (C-rate) in the **New label** text field.
- 9 Click OK.

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.
- 7 In the associated text field, type $\DELTA T (K)$.
- 8 Select the Secondary y-axis label check box.
- 9 In the associated text field, type Battery load (1).
- 10 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 1, 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

- I In the Model Builder window, right-click Probe Plot Group 2 and choose Table Graph.
- 2 In the Settings window for Table Graph, locate the Data section.
- 3 From the Plot columns list, choose Manual.
- 4 In the Columns list, select i_app/i_IC (I).
- 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 From the Legends list, choose Manual.
- 8 In the table, enter the following settings:

Legends

Battery load (C-rate)

9 Right-click Table Graph 2 and choose Rename.

10 In the Rename Table Graph dialog box, type Battery load in the New label text field.

II Click OK.

Temperature

- I In the Model Builder window, right-click Probe Table Graph I and choose Rename.
- 2 In the Rename Table Graph dialog box, type Temperature in the New label text field.
- 3 Click OK.
- 4 In the Probe Plot Group 2 toolbar, click **I** Plot.
- **5** Click the **Com Extents** button in the **Graphics** toolbar.

DEFINITIONS (COMP2)

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

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 Right-click Adjacent I and choose Rename.
- 9 In the Rename Adjacent dialog box, type Battery Surface in the New label text field.10 Click OK.

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 In the Results toolbar, click 🐐 Attributes 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.

Temperature and flow

- I In the **Results** toolbar, click **I 3D Plot Group**.
- 2 In the Settings window for 3D Plot Group, type Temperature and flow in the Label text field.
- 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 1

- 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) (sol1).
- 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. From the Color table list, choose ThermalLight.
- 7 In the **Temperature and flow** toolbar, click **I** 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) (sol1).
- 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 **I** Plot.
- **4** Click the |+ **Zoom Extents** button in the **Graphics** toolbar.

Load cycle

- I In the Model Builder window, right-click Probe Plot Group I and choose Rename.
- 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 two-way 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 two-way and one-way 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 two-way and oneway approaches are relatively close, while the one-way approach is much faster to solve.