

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

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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 (e.g. 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, $k_{T,ang}$, 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 $h = 20 \text{ W/(m}^2 \cdot \text{K})$ 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.

Results and Discussion



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

- I 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 \bigcirc Study.
- 7 In the Select Study tree, select General Studies>Time Dependent.
- 8 Click **M** Done.

GEOMETRY I

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

- I In the Geometry toolbar, click 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

- I In the Model Builder window, under Global Definitions click Parameters I.
- 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.

- I In the Home toolbar, click f(X) 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 Angular frequency text field, type 2*pi/cycle_time.

DEFINITIONS

Variables I

- I In the Home toolbar, click a= 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
Іарр	lb.I_1C*7.5*(wv1(t/ 1[s]))*(t<1500)	A	Applied current

Mean Temperature

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

- I 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

- I 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

- I 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

- 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 Home toolbar, click 🙀 Add Material to close the Add Material window.

MATERIALS

Steel AISI 4340 (mat1)

- I 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.

- I In the Model Builder window, under Component I (compl) 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 $Q_{cell,0}$ text field, type Q_batt.
- **6** In the $SOC_{cell,0}$ text field, type SOC_{init} .

Cell Equilibrium Potential I

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.

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

- I In the Model Builder window, click Voltage Losses I.
- 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 I (compl) click Heat Transfer in Solids (ht).

Solid 2

- I 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

- I 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

- I 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 Click the **Convective heat flux** button.
- **5** In the h text field, type 20.
- 6 In the T_{ext} text field, type T_init.

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_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 And Multiphysics Couplings and choose Domain> Electrochemical Heating.

MESH I

Mapped I

- I In the Mesh toolbar, click III 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 I and choose Build All.

The mesh should be as shown below:



STUDY I

Step 1: Time Dependent

- I In the Model Builder window, under Study I click Step I: 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 (soll)

I In the Study toolbar, click **here** 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 I (soll) node, then click Time-Dependent Solver I.
- 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 (Ib)

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

- I 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 (Ib)

- I In the Model Builder window, click Cell Potential and Load (lb).
- 2 In the Settings window for ID 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.

- I 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 \longleftrightarrow **Zoom Extents** button in the **Graphics** toolbar.

Temperature vs. Time

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

- I In the Model Builder window, under Results click Probe Plot Group 5.
- 2 In the Settings window for ID 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

- I 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

- I 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 Slank Model.

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 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 I

Rectangle 1 (r1)

I 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)

- I 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 (mcel)

- I 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

- I 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

- I 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 mcel, select Domain 3 only.

Mandrel

- I 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.

 $20\ |\$ thermal modeling of a cylindrical lithium-ion battery in 2d