



1D Lithium-Ion Battery for Thermal Models

Introduction

This model is used within the [Thermal Modeling of a Cylindrical Lithium-Ion Battery in 3D](#) and [Liquid-Cooled Lithium-Ion Battery Pack](#) examples to create an average heat source in an active battery material domain. See the model documentation of these two examples.

Model Definition

The 1D model has many similarities to the Application Library example [1D Isothermal Lithium-Ion Battery](#). The differences are the addition of negative and positive current collector domains and the use of a liquid electrolyte (1.2 M LiPF_6 in 3:7 EC:EMC) which also introduces a separator to the model. The cell model consists of the following five domains:


- Negative current collector (Al, 7 μm)
- Negative porous electrode (Li_xC_6 MCMB, 55 μm)
- Separator (30 μm)
- Positive porous electrode ($\text{Li}_y\text{Mn}_2\text{O}_4$, 55 μm)
- Positive current collector (Cu, 10 μm)

Application Library path: Battery_Design_Module/Thermal_Management/
li_battery_1d_for_thermal_models



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  **1D**.
- 2 In the **Select Physics** tree, select **Electrochemistry>Batteries>Lithium-Ion Battery (liion)**.
- 3 Click **Add**.
- 4 Click  **Done**.

GLOBAL DEFINITIONS

Parameters I



- 1 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_parameters.txt`.

GEOMETRY I

Interval I (il)


- 1 In the **Model Builder** window, under **Component I (comp1)** right-click **Geometry I** and choose **Interval**.
- 2 In the **Settings** window for **Interval**, locate the **Interval** section.
- 3 From the **Specify** list, choose **Interval lengths**.
- 4 In the table, enter the following settings:

Lengths (m)
L_neg
L_sep
L_pos


- 5 Click  **Build All Objects**.
- 6 Click the  **Zoom Extents** button in the **Graphics** toolbar.

DEFINITIONS

Negative Electrode

- 1 In the **Definitions** toolbar, click  **Explicit**.
- 2 Select Domain 1 only.
- 3 In the **Settings** window for **Explicit**, type Negative Electrode in the **Label** text field.



Positive Electrode

- 1 In the **Definitions** toolbar, click  **Explicit**.
- 2 Select Domain 3 only.
- 3 In the **Settings** window for **Explicit**, type Positive Electrode in the **Label** text field.

MATERIALS

This model uses battery materials available in the material library. Note: In the Materials node, c_{Eeqref} denotes the maximum lithium concentration in the active material.

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 **Battery>Electrolytes>LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery)**.
- 4 Click **Add to Component** in the window toolbar.
- 5 In the tree, select **Battery>Electrodes>Graphite, LixC6 MCMB (Negative, Li-ion Battery)**.
- 6 Click **Add to Component** in the window toolbar.
- 7 In the tree, select **Battery>Electrodes>LMO, LiMn2O4 Spinel (Positive, Li-ion Battery)**.
- 8 Click **Add to Component** in the window toolbar.
- 9 In the **Home** toolbar, click  **Add Material** to close the **Add Material** window.

MATERIALS

LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery) (mat1)

- 1 In the **Model Builder** window, under **Component 1 (comp1)>Materials** click **LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery) (mat1)**.
- 2 Select Domain 2 only.

Graphite, LixC6 MCMB (Negative, Li-ion Battery) (mat2)

- 1 In the **Model Builder** window, click **Graphite, LixC6 MCMB (Negative, Li-ion Battery) (mat2)**.
- 2 Select Domain 1 only.

LMO, LiMn2O4 Spinel (Positive, Li-ion Battery) (mat3)

- 1 In the **Model Builder** window, click **LMO, LiMn2O4 Spinel (Positive, Li-ion Battery) (mat3)**.
- 2 Select Domain 3 only.


LITHIUM-ION BATTERY (LIION)

Separator 1

- 1 In the **Model Builder** window, under **Component 1 (comp1)>Lithium-Ion Battery (liion)** click **Separator 1**.
- 2 In the **Settings** window for **Separator**, locate the **Porous Matrix Properties** section.

- 3 In the ϵ_1 text field, type `eps1_sep`.
- 4 Locate the **Effective Transport Parameter Correction** section. From the **Electrolyte conductivity** list, choose **User defined**. In the f_1 text field, type `eps1_sep^brug1_sep`.
- 5 From the **Diffusion** list, choose **User defined**. In the f_{D1} text field, type `eps1_sep^brug1_sep`.

Porous Electrode 1

- 1 In the **Physics** toolbar, click  **Domains** and choose **Porous Electrode**.
- 2 In the **Settings** window for **Porous Electrode**, locate the **Electrolyte Properties** section.
- 3 From the **Electrolyte material** list, choose **LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery) (mat1)**.
- 4 Locate the **Domain Selection** section. From the **Selection** list, choose **Negative Electrode**.
- 5 Locate the **Electrode Properties** section. In the σ_s text field, type `sigmas_neg`.
- 6 Locate the **Porous Matrix Properties** section. In the ϵ_s text field, type `epss_neg`.
- 7 In the ϵ_1 text field, type `eps1_neg`.

Particle Intercalation 1

- 1 In the **Model Builder** window, click **Particle Intercalation 1**.
- 2 In the **Settings** window for **Particle Intercalation**, locate the **Material** section.
- 3 From the **Particle material** list, choose **Graphite, LixC6 MCMB (Negative, Li-ion Battery) (mat2)**.
- 4 Locate the **Species Settings** section. In the $c_{s,init}$ text field, type `cs0_neg`.
- 5 Locate the **Particle Transport Properties** section. In the r_p text field, type `rp_neg`.
- 6 Click to expand the **Heat of Mixing** section. Select the **Include heat of mixing** check box.

Porous Electrode Reaction 1

- 1 In the **Model Builder** window, click **Porous Electrode Reaction 1**.
- 2 In the **Settings** window for **Porous Electrode Reaction**, locate the **Material** section.
- 3 From the **Material** list, choose **Graphite, LixC6 MCMB (Negative, Li-ion Battery) (mat2)**.
- 4 Locate the **Electrode Kinetics** section. In the $i_{0,ref}(T)$ text field, type `i0ref_neg`.


Porous Electrode 1

In the **Model Builder** window, click **Porous Electrode 1**.

Porous Matrix Double Layer Capacitance 1

In the **Physics** toolbar, click  **Attributes** and choose **Porous Matrix Double Layer Capacitance**.

Porous Electrode 2

- 1 In the **Physics** toolbar, click  **Domains** and choose **Porous Electrode**.
- 2 In the **Settings** window for **Porous Electrode**, locate the **Domain Selection** section.
- 3 From the **Selection** list, choose **Positive Electrode**.
- 4 Locate the **Electrolyte Properties** section. From the **Electrolyte material** list, choose **LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery) (mat1)**.
- 5 Locate the **Electrode Properties** section. In the σ_s text field, type `sigmas_pos`.
- 6 Locate the **Porous Matrix Properties** section. In the ϵ_s text field, type `eps_s_pos`.
- 7 In the ϵ_l text field, type `eps_l_pos`.
- 8 Locate the **Effective Transport Parameter Correction** section. From the **Electrolyte conductivity** list, choose **User defined**. In the f_l text field, type `eps_l_pos^brugl_pos`.
- 9 From the **Diffusion** list, choose **User defined**. In the f_{DI} text field, type `eps_l_pos^brugl_pos`.

Particle Intercalation 1

- 1 In the **Model Builder** window, click **Particle Intercalation 1**.
- 2 In the **Settings** window for **Particle Intercalation**, locate the **Material** section.
- 3 From the **Particle material** list, choose **LM0, LiMn2O4 Spinel (Positive, Li-ion Battery) (mat3)**.
- 4 Locate the **Species Settings** section. In the $c_{s,init}$ text field, type `cs0_pos`.
- 5 Locate the **Particle Transport Properties** section. In the r_p text field, type `rp_pos`.
- 6 Locate the **Heat of Mixing** section. Select the **Include heat of mixing** check box.

Porous Electrode Reaction 1

- 1 In the **Model Builder** window, click **Porous Electrode Reaction 1**.
- 2 In the **Settings** window for **Porous Electrode Reaction**, locate the **Material** section.
- 3 From the **Material** list, choose **LM0, LiMn2O4 Spinel (Positive, Li-ion Battery) (mat3)**.
- 4 Locate the **Electrode Kinetics** section. In the $i_{0,ref}(T)$ text field, type `i0ref_pos`.

Porous Electrode 2

In the **Model Builder** window, click **Porous Electrode 2**.


Porous Matrix Double Layer Capacitance 1

In the **Physics** toolbar, click  **Attributes** and choose **Porous Matrix Double Layer Capacitance**.


Electric Ground 1

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Electric Ground**.
- 2 Select Boundary 1 only.

Electrode Current Density 1

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Electrode Current Density**.
- 2 Select Boundary 4 only.
- 3 In the **Settings** window for **Electrode Current Density**, locate the **Electrode Current Density** section.
- 4 In the $i_{n,s}$ text field, type `i_app`.

Initial Values 2

- 1 In the **Physics** toolbar, click  **Domains** and choose **Initial Values**.
- 2 In the **Settings** window for **Initial Values**, locate the **Domain Selection** section.
- 3 From the **Selection** list, choose **Positive Electrode**.
- 4 Locate the **Initial Values** section. In the *phil* text field, type `-mat2.elpot.Eeq_int1(cs0_neg/mat2.elpot.cEeqref)`.
- 5 In the *cl* text field, type `c1_0`.
- 6 In the *phis* text field, type `mat3.elpot.Eeq_int1(cs0_pos/mat3.elpot.cEeqref)-mat2.elpot.Eeq_int1(cs0_neg/mat2.elpot.cEeqref)`.


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 *phil* text field, type `-mat2.elpot.Eeq_int1(cs0_neg/mat2.elpot.cEeqref)`.
- 4 In the *cl* text field, type `c1_0`.

DEFINITIONS (COMPI)

Set up the temperature value used in **Lithium-Ion Battery** interface.


Model Input 1

- 1 In the **Physics** toolbar, click  **Shared Properties** and choose **Model Input**.
- 2 In the **Settings** window for **Model Input**, locate the **Geometric Entity Selection** section.

- 3 From the **Selection** list, choose **All domains**.
- 4 Locate the **Definition** section. Click  **Select Quantity**.
- 5 In the **Physical Quantity** dialog box, type temperature in the text field.
- 6 Click  **Filter**.
- 7 In the tree, select **General>Temperature (K)**.
- 8 Click **OK**.


GLOBAL DEFINITIONS

Waveform I (wv1)

- 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 (COMPI)

Variables I

- 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
i_app	i_load*(wv1(t/1[s]))*(t<1500)		Applied current density

Domain Point Probe I


- 1 In the **Definitions** toolbar, click  **Probes** and choose **Domain Point Probe**.
- 2 In the **Settings** window for **Domain Point Probe**, locate the **Point Selection** section.
- 3 In row **Coordinate**, set **x** to L_neg+L_sep+L_neg.
- 4 Select the **Snap to closest point** check box.

Point Probe Expression I (ppb1)

- 1 In the **Model Builder** window, expand the **Domain Point Probe I** node, then click **Point Probe Expression I (ppb1)**.
- 2 In the **Settings** window for **Point Probe Expression**, type CellVoltageProbe in the **Variable name** text field.

- 3 Click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component I (comp I)>Lithium-Ion Battery>phis - Electric potential - V**.
- 4 Click to expand the **Table and Window Settings** section. Click  **Add Plot Window**.

Global Variable Probe I (var I)

- 1 In the **Definitions** toolbar, click  **Probes** and choose **Global Variable Probe**.
- 2 In the **Settings** window for **Global Variable Probe**, type CellCurrentProbe in the **Variable name** text field.
- 3 Locate the **Expression** section. In the **Expression** text field, type i_{app}/i_{10} .
- 4 Click to expand the **Table and Window Settings** section. From the **Plot window** list, choose **Probe Plot I**.

