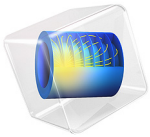

1D Isothermal Sodium-Ion Battery

Introduction

The sodium-ion battery (SIB) is an alternative to the lithium-ion battery (LIB). The SIB chemistry uses sodium ions instead of lithium ions for electrolyte charge transport and as redox species in the electrode reactions, with the advantage of sodium ions being more abundant and with a potentially smaller environmental footprint then lithium ions.

SIBs typically exhibit lower energy densities that LIBs, and hence constitute a candidate for replacing LIBs mainly in stationary applications. The SIB chemistry has many similarities to the LIB chemistry, and can often be described by the same equations for charge and mass transport, electrode kinetics, and electrode particle intercalation.

This example demonstrates how to use the Lithium-Ion Battery interface for modeling a SIB. The geometry is in one dimension (1D) and the model is isothermal. The discharge of a SIB for four different rates is studied.

Model Definition

This example models the battery cross section in 1D, which implies that edge effects in the length and height of the battery are neglected. The example uses the following three domains:

- Negative porous electrode: 64 μm
- Separator: 25 μm
- Positive porous electrode: 68 μm

The Lithium-Ion Battery interface, used for defining the model, accounts for:

- Electronic conduction in the electrodes
- Ionic charge transport in the electrodes and electrolyte/separator
- Material transport in the electrolyte, allowing for the introduction of the effects of concentration on the ionic conductivity and concentration overpotentials
- Material transport within the spherical particles that form the electrodes, defined on an extra (pseudo) dimension
- Butler–Volmer electrode kinetics using experimentally measured discharge curves for the equilibrium (half cell) potentials.

BOUNDARY CONDITIONS

For the electronic current balance, a potential of 0 V is set on the negative terminal using the Electric Ground boundary node. At the positive terminal, an average current density

is specified using the Electrode Current boundary node. The effect of contact resistances on both the negative and positive terminals are included. The inner boundaries facing the separator are insulating for electric currents.

For the ionic charge balance in the electrolyte, the terminal boundaries are insulating. Insulation boundary conditions also apply to the material balances at the terminal boundaries.

At the particle surface in the local particle model, the material flux is determined by the local electrochemical reaction rate.

BATTERY CHEMISTRY AND MATERIAL DEFINITIONS

The battery model consists of the following materials:

- Negative electrode: Hard Carbon HC (Li_xC_6)
- Positive electrode: NVPF ($Na_3V_2(PO_4)_2F_3$)
- Electrolyte: 1.0 M $NaPF_6$ dissolved in EC:PC (0.5:0.5 w/w)

User-defined interpolation functions are used for the equilibrium potentials, intercalation diffusion coefficients, and kinetic rate constants of the positive and negative electrode materials, and for the electrolyte salt diffusivity and electrolyte conductivity.

For complete details on the material properties and data, see Ref. 1 and Ref. 2.

Figure 1 displays the equilibrium potentials for the positive and negative electrode materials as functions of the measured state of sodiation (SOS).

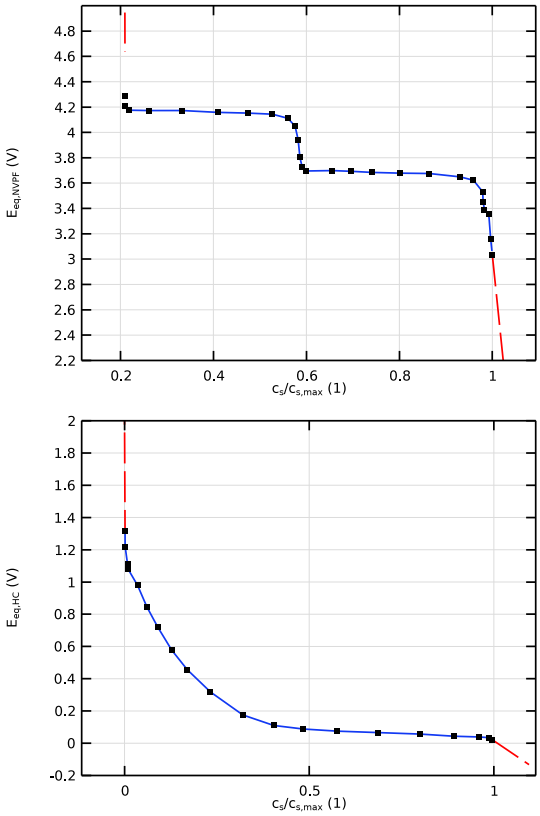

Figure 1: The equilibrium voltage of the positive electrode material (top) and the negative electrode material (bottom).

The model uses the following definition of the SOS:

$$\mathrm{SOS} = \frac{c_{s,\mathrm{Na}}^{\mathrm{surf}}}{c_{s,\mathrm{Na}}^{\mathrm{max}}}$$

Figure 2 displays the intercalation diffusion coefficients for the positive and negative electrode materials as functions of the solid concentration.

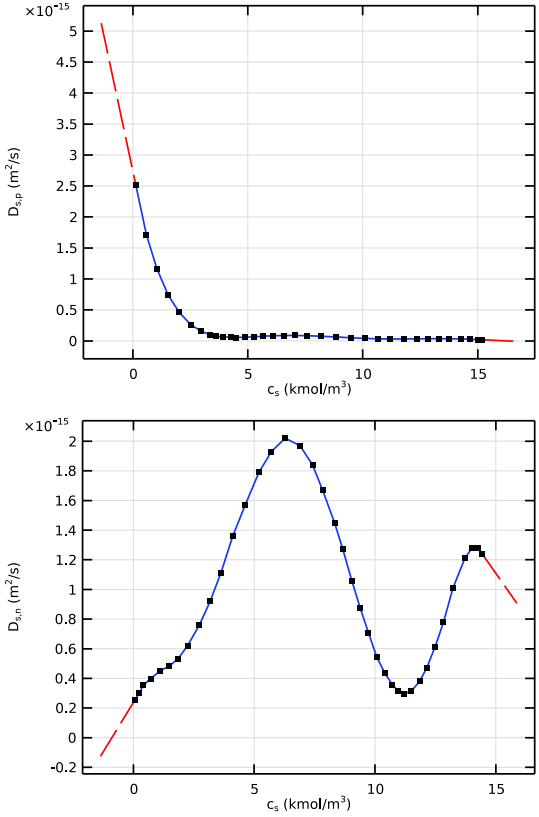

Figure 2: The intercalation diffusion coefficient of the positive electrode material (top) and the negative electrode material (bottom).

Figure 3 displays the kinetic rate constant for the positive and negative electrode materials as functions of the solid concentration.

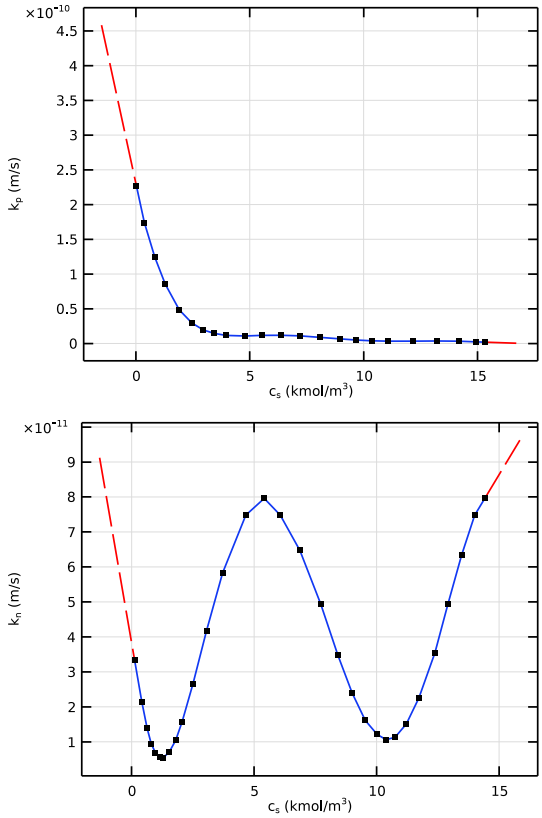

Figure 3: The kinetic rate constant of the positive electrode material (top) and the negative electrode material (bottom).

Figure 4 displays the electrolyte salt diffusivity and electrolyte conductivity as functions of the electrolyte salt concentration.

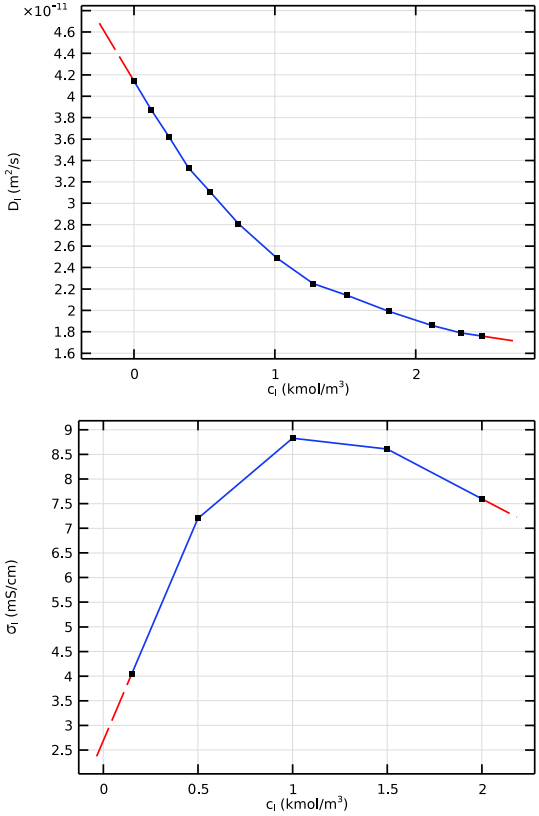

Figure 4: The electrolyte salt diffusivity (top) and the electrolyte conductivity (bottom).

Figure 5 shows the cell potential plotted as a function of the cell capacity, for four different discharge rates (1, 5, 10, and 12 A/m^2). This model defines end-of-discharge as the time when the cell voltage drops below 2 V.

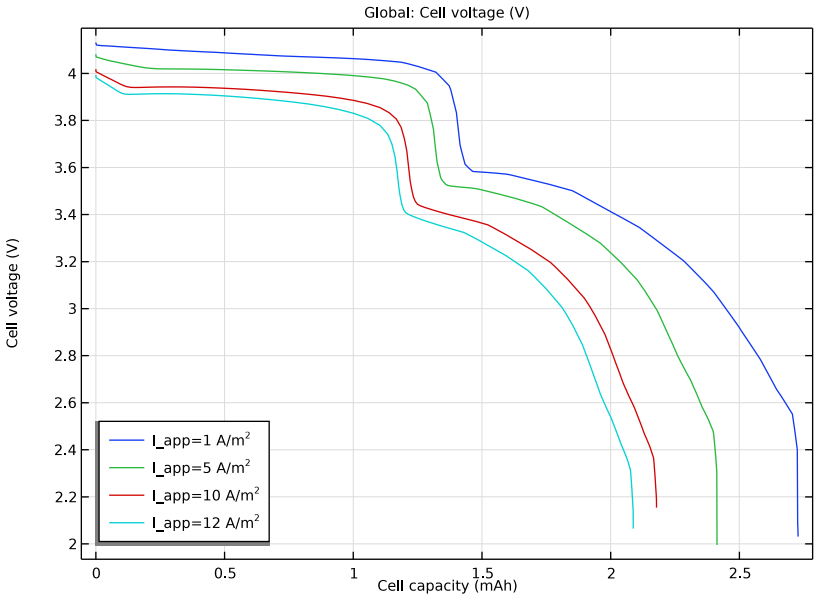

Figure 5: Cell voltage versus cell capacity.

Figure 6 and Figure 7 show the positive electrode potential and negative electrode potential, respectively, plotted as a function of the cell capacity, for the different discharge rates.

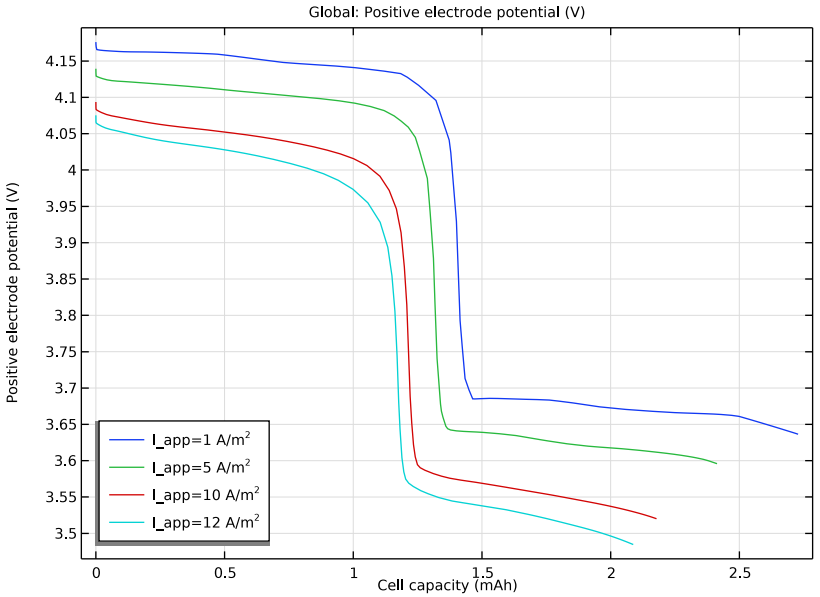

Figure 6: Positive electrode potential versus cell capacity.

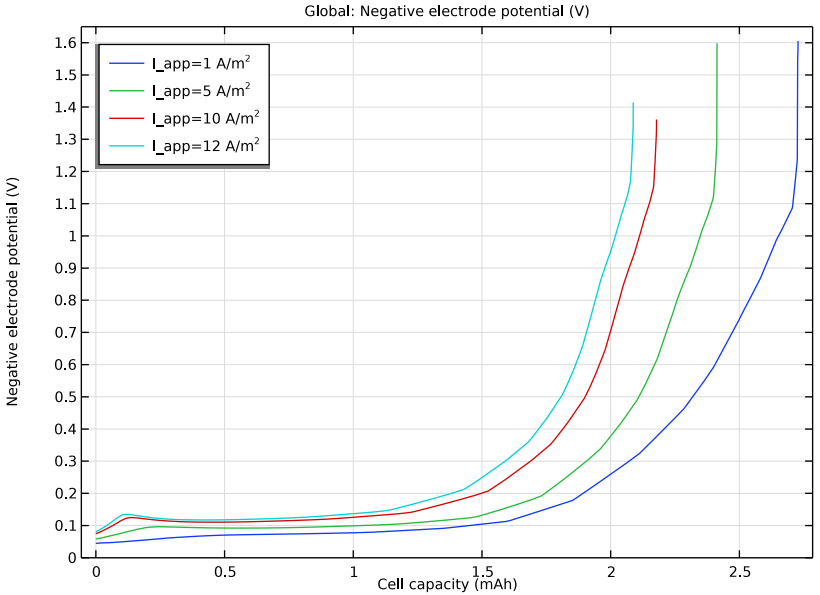

Figure 7: Negative electrode potential versus cell capacity.

References

1. K. Chayambuka, M. Jiang, G. Mulder, D.L. Danilov, and P.H.L. Notten, "Physics-based Modeling of Sodium-ion Batteries Part I: Experimental Parameter Determination", *Electrochim.Acta*, vol. 404, pp. 139726–139742, 2022.

2. K. Chayambuka, G. Mulder, D.L. Danilov, and P.H.L. Notten, "Physics-based Modeling of Sodium-ion Batteries Part II: Model and Validation", *Electrochim. Acta*, vol. 404, pp. 139764–139781, 2022.

Application Library path: `Battery_Design_Module/Batteries,_General/na_ion_battery_1d`

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 **Study**.

5 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces> Time Dependent with Initialization**.

(The **Time Dependent with Initialization study** will perform a time-dependent simulation, using an initialization study step to calculate the initial potentials in the cell.)

6 Click **Done**.

GLOBAL DEFINITIONS

Parameters 1

Load the parameters for this model from a text file.

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 `na_ion_battery_1d_parameters.txt`.

GEOMETRY 1

The geometry contains three domains. Create the geometry by specifying the lengths of the domains.

Interval 1 (i1)

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Geometry 1** 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_n
L_sep
L_p

5 Click **Build Selected**.

DEFINITIONS

The model uses $Na_3V_2(PO_4)_2F_3$ (NVPF) as the positive electrode material and hard carbon (HC) as the negative electrode material. 1M $NaPF_6$ dissolved in EC:PC (0.5:0.5 w/w) is used as the electrolyte.

Interpolation functions are used for the equilibrium potentials, intercalation diffusion coefficients and kinetic rate constants of the positive and negative electrode material, and for the electrolyte salt diffusivity and electrolyte conductivity. Refer to Figure 1, Figure 2, Figure 3 and Figure 4.

Set up the interpolation functions by importing the data from text files.

Interpolation - Eeq_NVPF (Positive Electrode)

1 In the **Home** toolbar, click f(x) **Functions** and choose **Local>Interpolation**.

2 In the **Settings** window for **Interpolation**, type `Interpolation - Eeq_NVPF (Positive Electrode)` in the **Label** text field.

3 Locate the **Definition** section. In the **Function name** text field, type `Eeq_NVPF`.

4 Click **Load from File**.

5 Browse to the model's Application Libraries folder and double-click the file `na_ion_battery_1d_Eeq_NVPF.txt`.

6 Locate the **Interpolation and Extrapolation** section. From the **Extrapolation** list, choose **Linear**.

7 Locate the **Units** section. In the **Function** table, enter the following settings:

Function	Unit
Eeq_NVPF	V

8 In the **Argument** table, enter the following settings:

Argument	Unit
t	1

Interpolation - Eeq_HC (Negative Electrode)

1 In the **Home** toolbar, click f(x) **Functions** and choose **Local>Interpolation**.

2 In the **Settings** window for **Interpolation**, type `Interpolation - Eeq_HC (Negative Electrode)` in the **Label** text field.

3 Locate the **Definition** section. In the **Function name** text field, type `Eeq_HC`.

4 Click **Load from File**.

5 Browse to the model's Application Libraries folder and double-click the file `na_ion_battery_1d_Eeq_HC.txt`.

6 Locate the **Interpolation and Extrapolation** section. From the **Extrapolation** list, choose **Linear**.

7 Locate the **Units** section. In the **Function** table, enter the following settings:

Function	Unit
Eeq_HC	V

8 In the **Argument** table, enter the following settings:

Argument	Unit
t	1

Interpolation - Ds_p

1 In the **Home** toolbar, click f(x) **Functions** and choose **Local>Interpolation**.

2 In the **Settings** window for **Interpolation**, type `Interpolation - Ds_p` in the **Label** text field.

3 Locate the **Definition** section. In the **Function name** text field, type `Ds_p`.

4 Click **Load from File**.

5 Browse to the model's Application Libraries folder and double-click the file `na_ion_battery_1d_Ds_p.txt`.

6 Locate the **Interpolation and Extrapolation** section. From the **Extrapolation** list, choose **Linear**.

7 Locate the **Units** section. In the **Function** table, enter the following settings:

Function	Unit
Ds_p	m^2/s

8 In the **Argument** table, enter the following settings:

Argument	Unit
t	kmol/m^3

Interpolation - Ds_n

1 In the **Home** toolbar, click f(x) **Functions** and choose **Local>Interpolation**.

2 In the **Settings** window for **Interpolation**, type `Interpolation - Ds_n` in the **Label** text field.

3 Locate the **Definition** section. In the **Function name** text field, type `Ds_n`.

4 Click **Load from File**.

5 Browse to the model's Application Libraries folder and double-click the file `na_ion_battery_1d_Ds_n.txt`.

6 Locate the **Interpolation and Extrapolation** section. From the **Extrapolation** list, choose **Linear**.

7 Locate the **Units** section. In the **Function** table, enter the following settings:

Function	Unit
Ds_n	m^2/s

8 In the **Argument** table, enter the following settings:

Argument	Unit
t	kmol/m^3

Interpolation - k_p

1 In the **Home** toolbar, click f(x) **Functions** and choose **Local>Interpolation**.

2 In the **Settings** window for **Interpolation**, type `Interpolation - k_p` in the **Label** text field.

3 Locate the **Definition** section. In the **Function name** text field, type `k_p`.

4 Click **Load from File**.

5 Browse to the model's Application Libraries folder and double-click the file `na_ion_battery_1d_k_p.txt`.

6 Locate the **Interpolation and Extrapolation** section. From the **Extrapolation** list, choose **Linear**.

7 Locate the **Units** section. In the **Function** table, enter the following settings:

Function	Unit
k_p	m/s

8 In the **Argument** table, enter the following settings:

Argument	Unit
t	kmol/m^3

Interpolation - k_n

1 In the **Home** toolbar, click f(x) **Functions** and choose **Local>Interpolation**.

2 In the **Settings** window for **Interpolation**, type `Interpolation - k_n` in the **Label** text field.

3 Locate the **Definition** section. In the **Function name** text field, type `k_n`.

4 Click **Load from File**.

5 Browse to the model's Application Libraries folder and double-click the file `na_ion_battery_1d_k_n.txt`.

6 Locate the **Interpolation and Extrapolation** section. From the **Extrapolation** list, choose **Linear**.

7 Locate the **Units** section. In the **Function** table, enter the following settings:

Function	Unit
k_n	m/s

8 In the **Argument** table, enter the following settings:

Argument	Unit
t	kmol/m^3

Interpolation - Dl

1 In the **Home** toolbar, click f(x) **Functions** and choose **Local>Interpolation**.

2 In the **Settings** window for **Interpolation**, type `Interpolation - Dl` in the **Label** text field.

3 Locate the **Definition** section. In the **Function name** text field, type `Dl`.

4 Click **Load from File**.

5 Browse to the model's Application Libraries folder and double-click the file `na_ion_battery_1d_Dl.txt`.

6 Locate the **Interpolation and Extrapolation** section. From the **Extrapolation** list, choose **Linear**.

7 Locate the **Units** section. In the **Function** table, enter the following settings:

Function	Unit
Dl	m^2/s

8 In the **Argument** table, enter the following settings:

Argument	Unit
t	kmol/m^3

Interpolation - sigmal

1 In the **Home** toolbar, click f(x) **Functions** and choose **Local>Interpolation**.

2 In the **Settings** window for **Interpolation**, type `Interpolation - sigmal` in the **Label** text field.

3 Locate the **Definition** section. In the **Function name** text field, type `sigmal`.

4 Click **Load from File**.

5 Browse to the model's Application Libraries folder and double-click the file `na_ion_battery_1d_sigmal.txt`.

6 Locate the **Interpolation and Extrapolation** section. From the **Extrapolation** list, choose **Linear**.

7 Locate the **Units** section. In the **Function** table, enter the following settings:

Function	Unit
sigmal	mS/cm

8 In the **Argument** table, enter the following settings:

Argument	Unit
t	kmol/m^3

Integration 1 (intop1)

Next, define two integration coupling operators that will be used to set up some post-processing variables. The variables are imported from a text file.

1 In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **Integration**.

2 In the **Settings** window for **Integration**, type `intop_ref_p` in the **Operator name** text field.

3 Locate the **Source Selection** section. From the **Geometric entity level** list, choose **Boundary**.

4 Select Boundary 3 only.

Integration 2 (intop2)

1 In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **Integration**.

2 In the **Settings** window for **Integration**, type `intop_ref_n` in the **Operator name** text field.

3 Locate the **Source Selection** section. From the **Geometric entity level** list, choose **Boundary**.

4 Select Boundary 2 only.

Variables 1

1 In the **Model Builder** window, right-click **Definitions** and choose **Variables**.

2 In the **Settings** window for **Variables**, locate the **Variables** section.

3 Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `na_ion_battery_1d_variables.txt`.

SODIUM-ION BATTERY

Set up the physics of the sodium-ion battery using the **Lithium-Ion Battery** Interface.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Lithium-Ion Battery (liion)**.

2 In the **Settings** window for **Lithium-Ion Battery**, type `Sodium-Ion Battery` in the **Label** text field.

3 Locate the **Cross-Sectional Area** section. In the A_c text field, type `Acc`.

Separator 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Sodium-Ion Battery (liion)** click **Separator 1**.

2 In the **Settings** window for **Separator**, locate the **Electrolyte Properties** section.

3 From the σ_l list, choose **User defined**. In the associated text field, type `sigmal(cl)`.

4 From the D_l list, choose **User defined**. In the associated text field, type `Dl(cl)`.

5 From the t_+ list, choose **User defined**. In the associated text field, type `tplus`.

6 From the $\mathrm{dln}f/\mathrm{dln}c_l$ list, choose **User defined**.

7 Locate the **Porous Matrix Properties** section. In the ε_l text field, type `epsl_sep`.

Porous Electrode 1

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

2 Select Domain 1 only.

3 In the **Settings** window for **Porous Electrode**, locate the **Electrolyte Properties** section.

4 From the σ_l list, choose **User defined**. In the associated text field, type `sigmal(cl)`.

5 From the D_l list, choose **User defined**. In the associated text field, type `Dl(cl)`.

6 From the t_+ list, choose **User defined**. In the associated text field, type `tplus`.

7 From the $\mathrm{dln}f/\mathrm{dln}c_l$ list, choose **User defined**.

8 Locate the **Electrode Properties** section. In the σ_s text field, type `sigmaeff_n`.

9 Locate the **Porous Matrix Properties** section. In the ε_s text field, type `1-epsf_n-epsl_n`.

10 In the ε_l text field, type `epsl_n`.

11 Locate the **Effective Transport Parameter Correction** section. From the **Electrical conductivity** list, choose **No correction**.

Particle Intercalation 1

1 In the **Model Builder** window, click **Particle Intercalation 1**.

2 In the **Settings** window for **Particle Intercalation**, locate the **Species Settings** section.

3 In the $c_{s,init}$ text field, type `cs_0_n`.

4 From the $c_{s,max}$ list, choose **User defined**. In the associated text field, type `csmax_n`.

5 Locate the **Particle Transport Properties** section. From the D_s list, choose **User defined**. In the associated text field, type `Ds_n(liion.cs_pce1)`.

6 In the r_p text field, type `R_n`.

7 Click to expand the **Operational SOCs for Initial Cell Charge Distribution** section. From the soc_{min} list, choose **User defined**. From the soc_{max} list, choose **User defined**.

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 **Equilibrium Potential** section.

3 From the E_{eq} list, choose **User defined**. In the associated text field, type `Eeq_HC(liion.cs_surface/csmax_n)`.

4 Locate the **Electrode Kinetics** section. From the **Exchange current density type** list, choose **Rate constant**.

5 In the k text field, type `k_n(liion.cs_surface)`.

6 In the α_a text field, type `alpha`.

7 In the α_c text field, type `1-alpha`.

8 In the $c_{l,ref}$ text field, type `cl_ref`.

9 Click to expand the **Heat of Reaction** section. From the list, choose **User defined**.

Porous Electrode 2

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

2 Select Domain 3 only.

3 In the **Settings** window for **Porous Electrode**, locate the **Electrolyte Properties** section.

4 From the σ_l list, choose **User defined**. In the associated text field, type `sigmal(cl)`.

5 From the D_l list, choose **User defined**. In the associated text field, type `Dl(cl)`.

6 From the t_+ list, choose **User defined**. In the associated text field, type `tplus`.

7 From the $\mathrm{dln}f/\mathrm{dln}c_l$ list, choose **User defined**.

8 Locate the **Electrode Properties** section. In the σ_s text field, type `sigmaeff_p`.

9 Locate the **Porous Matrix Properties** section. In the ε_s text field, type `1-epsf_p-epsl_p`.

10 In the ε_l text field, type `epsl_p`.

11 Locate the **Effective Transport Parameter Correction** section. From the **Electrical conductivity** list, choose **No correction**.

Particle Intercalation 1

1 In the **Model Builder** window, click **Particle Intercalation 1**.

2 In the **Settings** window for **Particle Intercalation**, locate the **Species Settings** section.

3 In the $c_{s,init}$ text field, type `cs_0_p`.

4 From the $c_{s,max}$ list, choose **User defined**. In the associated text field, type `csmax_p`.

5 Locate the **Particle Transport Properties** section. From the D_s list, choose **User defined**. In the associated text field, type `Ds_p(liion.cs_pce2)`.

6 In the r_p text field, type `R_p`.

7 Locate the **Operational SOCs for Initial Cell Charge Distribution** section. From the soc_{min} list, choose **User defined**. From the soc_{max} list, choose **User defined**.

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 **Equilibrium Potential** section.

3 From the E_{eq} list, choose **User defined**. In the associated text field, type `Eeq_NVPF(liion.cs_surface/csmax_p)`.

4 Locate the **Electrode Kinetics** section. From the **Exchange current density type** list, choose **Rate constant**.

5 In the k text field, type `k_p(liion.cs_surface)`.

6 In the α_a text field, type `alpha`.

7 In the α_c text field, type `1-alpha`.

8 In the $c_{l,ref}$ text field, type `cl_ref`.

9 Locate the **Heat of Reaction** section. From the list, choose **User defined**.

Electric Ground 1

Set up the boundary conditions. The negative terminal is grounded. Also include a contact resistance.

1 In the **Physics** toolbar, click **Boundaries** and choose **Electric Ground**.

2 Select Boundary 1 only.

3 In the **Settings** window for **Electric Ground**, locate the **Contact Resistance** section.

4 Select the **Include contact resistance** check box.

5 In the R_c text field, type `Rct_n`.

Electrode Current 1

Set up a current at the positive terminal. Also include a contact resistance.

1 In the **Physics** toolbar, click **Boundaries** and choose **Electrode Current**.

2 Select Boundary 4 only.

3 In the **Settings** window for **Electrode Current**, locate the **Electrode Current** section.

4 From the list, choose **Average current density**.

5 In the $i_{s,average}$ text field, type `-I_app`.

6 In the $\phi_{s,bnd,init}$ text field, type `4.2[V]`.

7 Locate the **Contact Resistance** section. Select the **Include contact resistance** check box.

8 In the R_c text field, type `Rct_p`.

Initial Values 1

Set up the initial electrolyte concentration. The initial potentials in the cell are automatically calculated by the **Current Distribution Initialization** study step.

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 *cl* text field, type `cl_0`.

GLOBAL DEFINITIONS

Default Model Inputs

Set up the temperature value used in the entire model.

1 In the **Model Builder** window, under **Global Definitions** click **Default Model Inputs**.

2 In the **Settings** window for **Default Model Inputs**, locate the **Browse Model Inputs** section.

3 In the tree, select **General>Temperature (K) - minput.T**.

4 Find the **Expression for remaining selection** subsection. In the **Temperature** text field, type `T0`.

STUDY 1

Set up a **Parametric Sweep** to study four different discharge rates.

Parametric Sweep

1 In the **Study** toolbar, click **Parametric Sweep**.

2 In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.

3 Click **Add**.

4 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
I_app (Applied current density)	`1 5 10 12`	`A/m^2`

Step 2: Time Dependent

1 In the **Model Builder** window, click **Step 2: Time Dependent**.

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

3 In the **Output times** text field, type `range(0,0.1*T_dch, T_dch)`.

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

5 In the **Relative tolerance** text field, type `0.0001`.

Solution 1 (sol1)

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

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 **Store every Nth step** text field, type `5`.

Add a **Stop Condition** to stop the solver if the cell voltage drops below 2.0 V.

6 Right-click **Study 1>Solver Configurations>Solution 1 (sol1)>Time-Dependent Solver 1** and choose **Stop Condition**.

7 In the **Settings** window for **Stop Condition**, locate the **Stop Expressions** section.

8 Click + **Add**.

9 In the table, enter the following settings:

Stop expression	Stop if	Active	Description
`comp1.E_cell<2[V]`	True (>=1)	√	`Stop expression 1`

10 Locate the **Output at Stop** section. From the **Add solution** list, choose **Step after stop**.

11 Clear the **Add warning** check box.

12 In the **Study** toolbar, click = **Compute**.

RESULTS

Some plots are created by default. Additionally, add plots for the cell potential versus cell capacity (Figure 5), positive electrode potential versus cell capacity (Figure 6), and negative electrode potential versus cell capacity (Figure 7).

Cell Voltage vs. Cell Capacity

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

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

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/ Parametric Solutions 1 (sol3)**.

Global 1

1 Right-click **Cell Voltage vs. Cell Capacity** and choose **Global**.

2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.

3 In the table, enter the following settings:

Expression	Unit	Description
`E_cell`	`V`	`Cell voltage`

4 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Definitions>Variables>E_cell - Cell voltage - V**.

5 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

6 In the **Expression** text field, type `t*I_app*Acc`.

7 From the **Unit** list, choose **mAh**.

8 Select the **Description** check box. In the associated text field, type `Cell capacity`.

9 Click to expand the **Legends** section. Find the **Include** subsection. Clear the **Description** check box.

Cell Voltage vs. Cell Capacity

1 In the **Model Builder** window, click **Cell Voltage vs. Cell Capacity**.

2 In the **Settings** window for **1D Plot Group**, locate the **Legend** section.

3 From the **Position** list, choose **Lower left**.

4 In the **Cell Voltage vs. Cell Capacity** toolbar, click **Plot**.

5 Right-click **Cell Voltage vs. Cell Capacity** and choose **Duplicate**.

Positive Electrode Potential vs. Cell Capacity

1 In the **Model Builder** window, under **Results** click **Cell Voltage vs. Cell Capacity 1**.

2 In the **Settings** window for **1D Plot Group**, type `Positive Electrode Potential vs. Cell Capacity` in the **Label** text field.

Global 1

1 In the **Model Builder** window, expand the **Positive Electrode Potential vs. Cell Capacity** node, then click **Global 1**.

2 In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Definitions> Variables>E_pos - Positive electrode potential - V**.

Positive Electrode Potential vs. Cell Capacity

1 In the **Model Builder** window, click **Positive Electrode Potential vs. Cell Capacity**.

2 In the **Positive Electrode Potential vs. Cell Capacity** toolbar, click **Plot**.

3 Right-click **Positive Electrode Potential vs. Cell Capacity** and choose **Duplicate**.

Negative Electrode Potential vs. Cell Capacity

1 In the **Model Builder** window, under **Results** click **Positive Electrode Potential vs. Cell Capacity 1**.

2 In the **Settings** window for **1D Plot Group**, type `Negative Electrode Potential vs. Cell Capacity` in the **Label** text field.

Global 1

1 In the **Model Builder** window, expand the **Negative Electrode Potential vs. Cell Capacity** node, then click **Global 1**.

2 In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Definitions> Variables>E_neg - Negative electrode potential - V**.

Negative Electrode Potential vs. Cell Capacity

1 In the **Model Builder** window, click **Negative Electrode Potential vs. Cell Capacity**.

2 In the **Settings** window for **1D Plot Group**, locate the **Legend** section.

3 From the **Position** list, choose **Upper left**.

4 In the **Negative Electrode Potential vs. Cell Capacity** toolbar, click **Plot**.