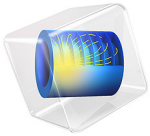

# 1D Isothermal Lithium–Air Battery

## *Introduction*

Metal-air batteries have an especially high specific energy density. Lithium–air batteries have a theoretical energy density value of about 11,400 Wh/kg, which is nearly 10 times greater than the lithium-ion batteries. Such an increase in capacity versus conventional lithium-ion batteries would be useful in many applications. However, there are many challenges in realizing a practical lithium-air battery.

A unit cell of a lithium–air battery typically consists of a thin lithium sheet as the negative electrode, a porous carbon electrode filled with oxygen/air as the positive electrode, and a separator material between the electrodes. The organic electrolyte used consists of a dissolved lithium salt in an aprotic solvent. The oxidation of lithium at the anode and reduction of oxygen at the cathode induces a current flow.

In this model example, discharge of a lithium–air battery (Ref. 1) is simulated using the Lithium-Ion Battery interface. The transport of oxygen (from external air) in the porous carbon electrode is modeled using the Transport of Diluted Species in Porous Media interface. The electrochemical reaction of oxygen reduction in the carbon electrode leads to changes in concentration of the reaction product and electrode porosity. In this example, model analysis is done for a range of discharge current densities. A comparison of the oxygen concentration, porosity, and film thickness in the positive electrode at low and high discharge current densities is done to understand their effect on the cell voltage profiles. This model can be used for studying the performance of lithium–air batteries and for providing insights toward cell design.

## *Model Definition*

A 1D isothermal cell model for lithium–air battery is presented. Figure 1 shows the 1D model geometry. It consists of two domains: the separator and the positive porous carbon electrode filled with oxygen. The lithium metal negative electrode is modeled as a boundary. The unit cell is filled with an organic electrolyte solution.

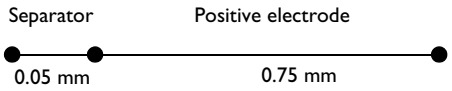


*Figure 1: 1D model geometry of a lithium–air unit cell.*

## ELECTROCHEMICAL REACTIONS

The porous carbon electrode provides a site for the electrochemical reduction of oxygen. During operation, oxygen from the external air dissolves in the electrolyte, moves through the pores of the positive electrode and reacts with lithium ions at the active site. The reaction considered at the positive electrode is

$$2Li^+ + O_2 + 2e^- \rightarrow Li_2O_2 \qquad E_{eq} = 2.96\,V \tag{1}$$

The reaction product ($Li_2O_2$) in the positive electrode is insoluble in the organic electrolyte (beyond its solubility limit in the electrolyte) and deposits as a film on the active surface area in the porous electrode. The kinetic expression for the electrode reaction above is

$$i_{loc} = nF\left\{k_a c_{Li_2O_2}\exp\left(\frac{0.5nF\eta}{RT}\right) - k_c (c_{Li^+})^2 c_{O_2}\exp\left(\frac{-0.5nF\eta}{RT}\right)\right\} \tag{2}$$

where $i_{loc}$ is the local current density, $n$ is the number of electrons transferred, $\eta$ is the overpotential, $k_a$ is the anodic transfer coefficient, $k_c$ is the cathodic transfer coefficient, and $c_i$ is the concentration of species $i$ at the active site.

The overpotential $\eta$ for the reaction is calculated from the electrode potential ($\phi_s$), the electrolyte potential ($\phi_l$), the potential drop due to the particle film resistance ($\Delta\phi_{film}$), and the equilibrium potential of the reaction ($E_{eq}$), as follows.

$$\eta = \phi_s - \phi_l - \Delta\phi_{film} - E_{eq} \tag{3}$$

The potential drop due to the particle film resistance is given as

$$\Delta\phi_{film} = i_{loc} R_{film} \varepsilon_{Li_2O_2} \tag{4}$$

where $R_{film}$ is the electrical resistivity across the $Li_2O_2$ film and $\varepsilon_{Li2O2}$ is the volume fraction of solid $Li_2O_2$.

The reaction considered in the negative electrode is

$$Li \rightarrow Li^+ + e^- \qquad E_{eq} = 0V \tag{5}$$

Lithium metal kinetics is used for this reaction at the negative electrode.

## PHYSICS SETUP

The Lithium-Ion Battery interface describes the following processes:

- Electronic current conduction in the electrodes

- Ionic charge transport in the electrolyte present in the porous electrodes and separator
- Material transport in the electrolyte present in the porous electrodes and separator
- Electrochemical reaction kinetics in the porous electrodes

In the positive electrode, spherical nonintercalating particles with concentration dependent electrode kinetics are used in the Lithium-Ion Battery interface. The thin lithium sheet (negative electrode) is represented using the Electrode Surface node with lithium metal electrode kinetics. The Bruggeman correction is used for the all the effective transport properties in the positive porous electrode and the separator.

The Transport of Diluted Species in Porous Media interface describes the mass transport of oxygen in the porous carbon positive electrode by diffusion, along with the consumption of oxygen due to the electrochemical reaction (Equation 1).

The change in the concentration of the reaction product ($Li_2O_2$) in the solution phase of the positive electrode is given as

$$\frac{\partial(\varepsilon_l c_{Li_2O_2})}{\partial t} = \frac{-1}{2F} a i_{loc} \times (c_{Li_2O_2} < c_{max,Li_2O_2}) \quad (6)$$

where $\varepsilon_l$ is the porosity and $a$ is the active specific surface area, respectively, of the positive electrode, and $c_{max,Li2O2}$ is the solubility limit of $Li_2O_2$ dissolved in the electrolyte. Note that $\varepsilon_l$ remains at the initial porosity value until the solubility limit of $Li_2O_2$ in the electrolyte is reached. The Domain ODEs and DAEs interface is used for modeling the changes in concentration of the reaction product in the solution phase of the positive electrode.

Beyond its solubility limit in the electrolyte, the reaction product ($Li_2O_2$) in the positive electrode deposits as a film on the active surface area. The change in the concentration of solid $Li_2O_2$, $c_{s,Li2O2}$, in the positive electrode is given as

$$\frac{\partial c_{s,Li_2O_2}}{\partial t} = \frac{1}{2F} a i_{loc} \times (c_{Li_2O_2} \geq c_{max,Li_2O_2}) \quad (7)$$

The porosity change due to solid $Li_2O_2$ deposition in the positive electrode is given as

$$\varepsilon_{Li_2O_2} = (c_{s,\,Li_2O_2} - c_{s0,\,Li_2O_2}) \times \frac{MW_{Li_2O_2}}{\rho_{Li_2O_2}} \quad (8)$$

where $c_{s0,Li2O2}$, $MW_{Li2O2}$, and $\rho_{Li2O2}$ are the initial concentration, molecular weight, and density of solid $Li_2O_2$ in the film, respectively. The Dissolving-Depositing Species section

of the Porous Electrode node is used to solve for the changes in concentration of the solid reaction product and electrode porosity in the positive porous electrode.

The active specific surface area of the positive porous electrode is determined by the morphology and the dynamic change of porosity due to solid $Li_2O_2$ film formation. The effective local surface area per unit volume of the electrode is given by,

$$a = a_0\left(1 - \left(\frac{\varepsilon_{Li_2O_2}}{\varepsilon_{l,0}}\right)^{0.5}\right) \tag{9}$$

where $\varepsilon_{l,0}$ is the initial porosity and $a_0$ is the initial active specific surface area, respectively, of the positive electrode. The value of 0.5 is related to the morphological shape of the solid $Li_2O_2$ reaction product.

### BOUNDARY CONDITIONS

The negative electrode (lithium metal) is set to a potential of 0 V (electric ground condition). At the positive electrode current collector boundary, a discharge current density is applied. A parametric study is performed for discharge current densities ranging from 0.05 $mA/cm^2$ to 0.5 $mA/cm^2$. The study includes a stop condition with a minimum voltage of 2.5 V.

Figure 2 shows the cell voltage profiles plotted as a function of capacity for different values of the discharge current density. At higher current densities, the discharge voltage and cell capacity are lower, as expected.

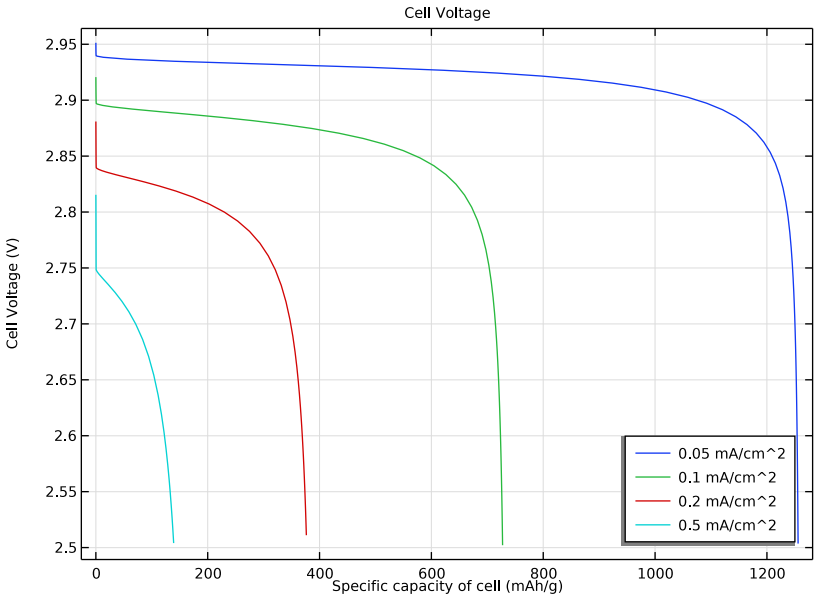


*Figure 2: Cell voltage profiles as a function of specific capacity of the cell for different values of the applied discharge current density.*

Figure 3 and Figure 4 show the oxygen concentration in the positive porous electrode at different times (discharge states of the battery), for a low and high value of the discharge current density, respectively. The decreased transport of oxygen in the positive electrode at high discharge currents, as seen in Figure 4, leads to the loss in capacity at high

discharge rates. The electrochemical reaction of oxygen reduction is limited to regions close to the positive electrode/current collector edge, as the discharge rate increases.

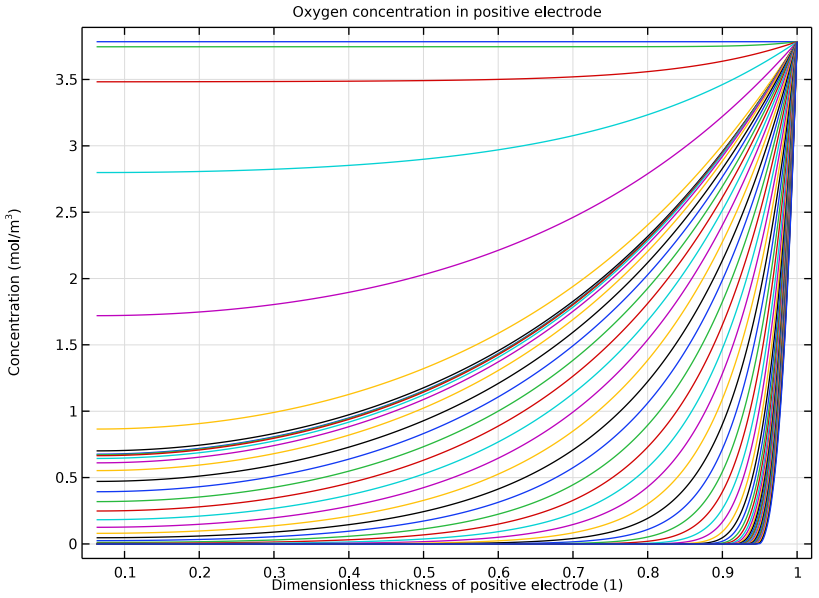


*Figure 3: Variation of oxygen concentration in the positive electrode at different times (discharge states of the battery), for a low value of the discharge current density.*

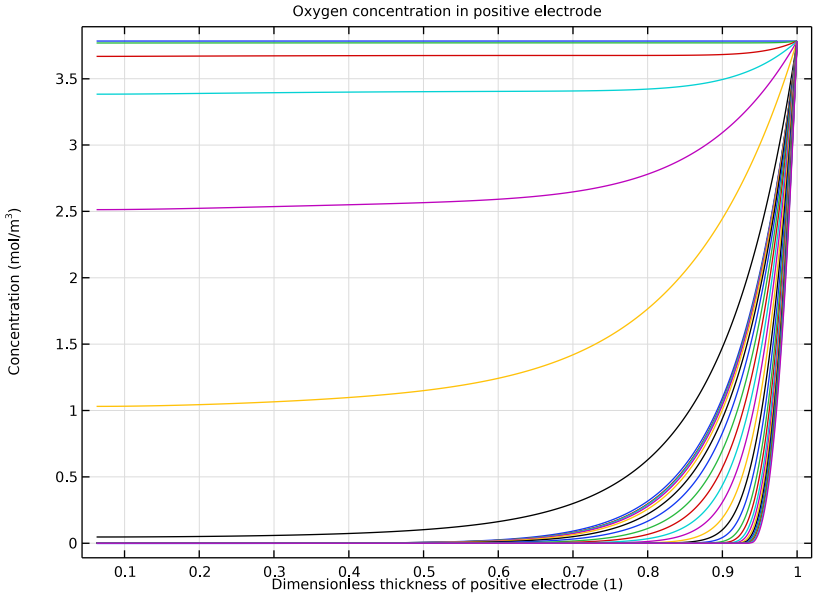


*Figure 4: Variation of oxygen concentration in the positive electrode at different times (discharge states of the battery), for a high value of the discharge current density.*

Figure 5 and Figure 6 similarly show the variation of the volume fraction of $Li_2O_2$ in the positive electrode at different times, for a low and high value of the discharge current density, respectively. At high discharge rates, the $Li_2O_2$ deposition on the active surface

area of the porous carbon electrode is predominantly limited to regions close to the positive electrode/current collector edge, as seen in Figure 6.

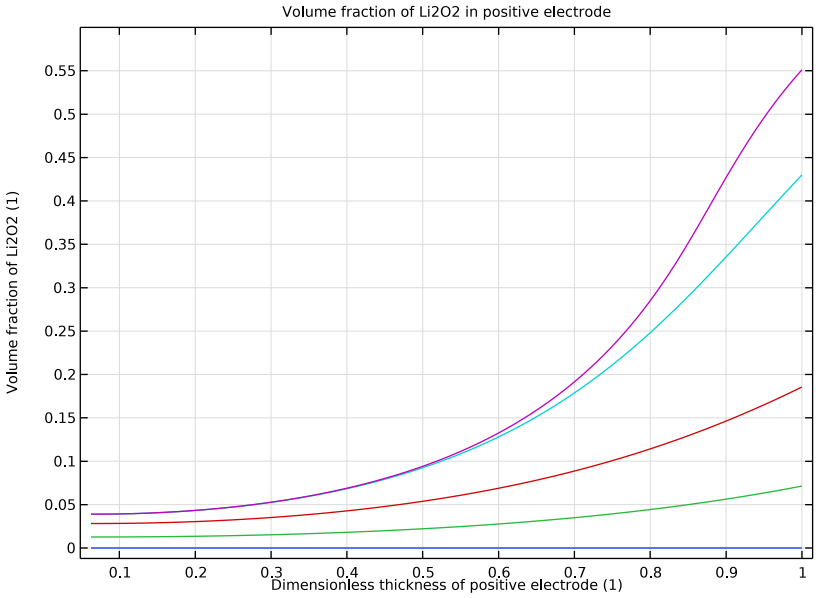


*Figure 5: Variation of volume fraction of $Li_2O_2$ in the positive electrode at different times (discharge states of the battery), for a low value of the discharge current density.*

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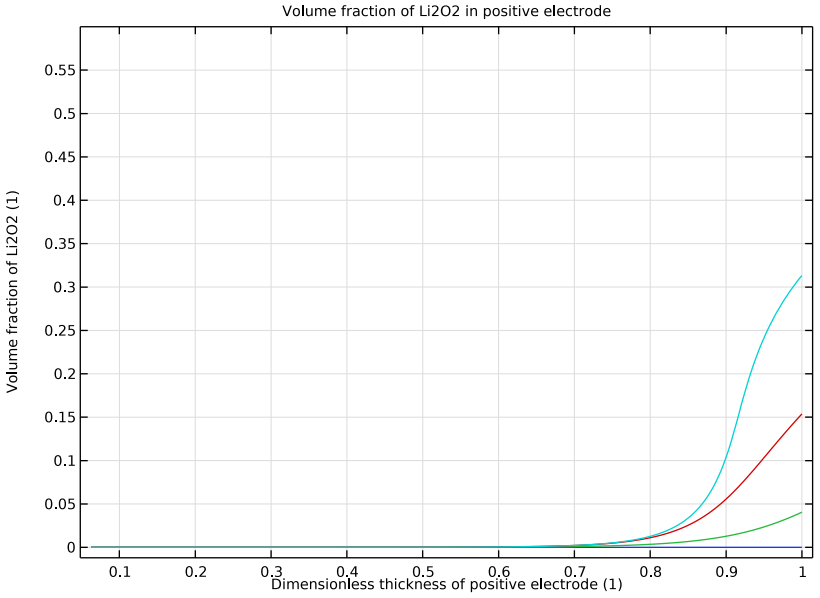


*Figure 6: Variation of volume fraction of $Li_2O_2$ in the positive electrode at different times (discharge states of the battery), for a high value of the discharge current density.*

Figure 7 and Figure 8 similarly show the variation of porosity in the positive electrode at different times, for a low and high value of the discharge current density, respectively. The porosity of the porous carbon electrode decreases predominantly at regions close to the positive electrode/current collector edge at high discharge current densities, as seen in

Figure 8. Incomplete utilization of the porous carbon electrode at high discharge rates leads to lower cell capacities at high rates as seen in Figure 2.

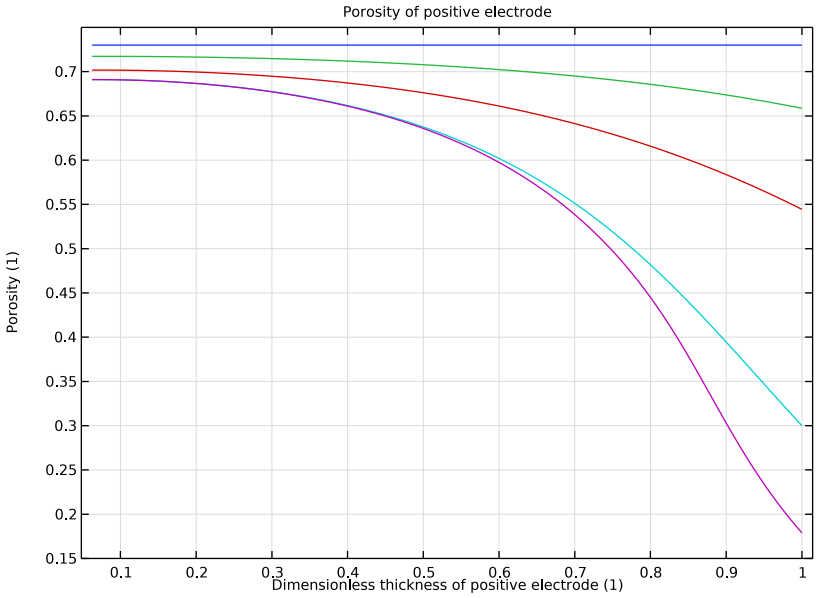


*Figure 7: Variation of porosity in the positive electrode at different times (discharge states of the battery), for a low value of the discharge current density.*

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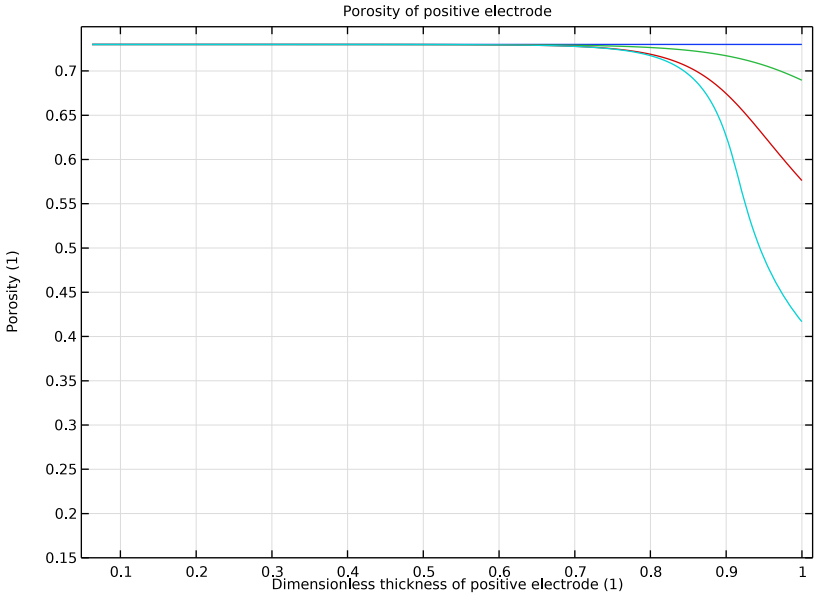


*Figure 8: Variation of porosity in the positive electrode at different times (discharge states of the battery), for a high value of the discharge current density.*

## *Reference*

1. U. Sahapatsombut, H. Cheng, and K. Scott, "Modeling the micro-macro homogeneous cycling behavior of a lithium-air battery," *Journal of Power Sources*, vol. 227, pp. 243–253, 2013.

**Application Library path:** `Battery_Design_Module/Batteries,_Lithium-Ion/li_air_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**.

Add a Lithium-Ion Battery interface, a Transport of Diluted Species in Porous Media interface, and Domain ODEs and DAEs interface. The Transport of Diluted Species in Porous Media interface is used for modeling the transport of oxygen (from external air) in the porous carbon electrode. The Domain ODEs and DAEs interface is used for modeling the changes in concentration of the reaction product in the solution phase of the positive electrode.

2 In the **Select Physics** tree, select **Electrochemistry>Batteries>Lithium-Ion Battery (liion)**.

3 Click **Add**.

4 In the **Electrolyte salt concentration (mol/m³)** text field, type `cLi`.

5 In the **Select Physics** tree, select **Chemical Species Transport> Transport of Diluted Species in Porous Media (tds)**.

6 Click **Add**.

7 In the **Concentrations (mol/m³)** table, enter the following settings:

| |
|---|
| c02 |

8 In the **Select Physics** tree, select **Mathematics>ODE and DAE Interfaces> Domain ODEs and DAEs (dode)**.

9 Click **Add**.

10 In the **Dependent variables (1)** table, enter the following settings:

| |
|---|
| ecLi2O2 |

11 Click  **Select Dependent Variable Quantity**.

12 In the **Physical Quantity** dialog box, type `concentration` in the text field.

13 Click  **Filter**.

14 In the tree, select **General>Concentration (mol/m^3)**.

15 Click **OK**.

16 In the **Model Wizard** window, click  **Select Source Term Quantity**.

17 In the **Physical Quantity** dialog box, type `reactionrate` in the text field.

18 Click  **Filter**.

19 In the tree, select **Transport>Reaction rate (mol/(m^3*s))**.

20 Click **OK**.

21 In the **Model Wizard** window, click **Study**.

22 In the **Select Study** tree, select **General Studies>Time Dependent**.

23 Click **Done**.

### GLOBAL DEFINITIONS

Load model parameters from a text file.

*Parameters 1*

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

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

3 Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `li_air_battery_1d_parameters.txt`.

### GEOMETRY 1

The geometry contains two domains, the separator and the positive porous electrode. Create the geometry by specifying the coordinates of the boundaries.

*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) |
|---|
| Lsep |
| Lpos |

5 In the **Home** toolbar, click **Build All**.

### DEFINITIONS

Load the model variables from a text file.

*Variables 1*

1 In the **Home** toolbar, click **Variables** and choose **Local Variables**.

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

3 From the **Geometric entity level** list, choose **Domain**.

4 Select Domain 2 only.

5 Locate the **Variables** section. Click **Load from File**.

6 Browse to the model's Application Libraries folder and double-click the file `li_air_battery_1d_variables.txt`.

*Integration 1 (intop1)*

A boundary integration variable can be used to access the cell voltage at the end terminal during the computation.

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

2 In the **Settings** window for **Integration**, type `EndTerminal` 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.

### LITHIUM-ION BATTERY (LIION)

Set up the physics in the battery interface starting with the separator and the positive porous electrode. The lithium metal negative electrode is modeled using the Electrode Surface condition with lithium metal electrode kinetics.

*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 **Electrolyte Properties** section.

3 From the $\sigma_l$ list, choose **User defined**. In the associated text field, type `kappaLi`.

4 From the $D_l$ list, choose **User defined**. In the associated text field, type `DLi`.

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**. In the associated text field, type `dlnfdlnc`.

7 Locate the **Porous Matrix Properties** section. In the $\varepsilon_l$ text field, type `epsilonsep`.

*Porous Electrode 1*

Set up the positive electrode parameters. Use Dissolving-Depositing Species formulation for modeling the change in porosity of the positive electrode.

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

2 Select Domain 2 only.

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

4 From the $\sigma_l$ list, choose **User defined**. In the associated text field, type `kappaLi`.

5 From the $D_l$ list, choose **User defined**. In the associated text field, type `DLi`.

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**. In the associated text field, type `dlnfdlnc`.

8 Locate the **Electrode Properties** section. In the $\sigma_s$ text field, type `Kpos`.

9 Locate the **Particle Properties** section. From the list, choose **Nonintercalating particles**.

10 Locate the **Porous Matrix Properties** section. In the $\varepsilon_s$ text field, type `epsilons0`.

11 In the $\varepsilon_l$ text field, type `epsilonl0`.

12 Click to expand the **Dissolving-Depositing Species** section. Click + **Add**.

13 In the table, enter the following settings:

| Species | Density (kg/m^3) | Molar mass (kg/mol) |
|---|---|---|
| s1 | rhoLi2O2 | MLi2O2 |

14 Clear the **Add volume change to electrode volume fraction** check box.

15 Click to expand the **Film Resistance** section. From the **Film resistance** list, choose **Surface resistance**.

16 In the $R_{\mathrm{film}}$ text field, type `Rfilm*epsilonLi2O2`.

*Porous Electrode Reaction 1*

Set up the porous electrode reaction parameters. Beyond its solubility limit in the electrolyte, the reaction product (Li2O2) in the positive electrode deposits as a film on the active surface area.

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 $E_{\mathrm{eq}}$ list, choose **User defined**. In the associated text field, type `Eeq`.

4 Locate the **Electrode Kinetics** section. From the **Kinetics expression type** list, choose **Concentration dependent kinetics**.

5 In the $i_0$ text field, type `1`.

6 In the $\alpha_a$ text field, type `0.5*n`.

7 In the $\alpha_c$ text field, type `0.5*n`.

8 In the $C_R$ text field, type `CRpos`.

9 In the $C_O$ text field, type `COpos`.

10 Locate the **Active Specific Surface Area** section. From the **Active specific surface area** list, choose **User defined**. In the $a_v$ text field, type `apos`.

11 Locate the **Stoichiometric Coefficients** section. In the $n$ text field, type `n`.

12 In the $\nu_{Li+}$ text field, type `-2`.

13 In the **Stoichiometric coefficients for dissolving-depositing species:** table, enter the following settings:

| Species | Stoichiometric coefficient (1) |
|---|---|
| s1 | 1*(cLi2O2>=cmaxLi2O2) |

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

*Electrode Surface 1*

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

2 Select Boundary 1 only.

*Electrode Reaction 1*

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

2 In the **Settings** window for **Electrode Reaction**, locate the **Equilibrium Potential** section.

3 From the $E_{eq}$ list, choose **User defined**. Locate the **Electrode Kinetics** section. In the $i_{0,ref}(T)$ text field, type `i0refLi`.

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

*Electrode Current Density 1*

Set up a current density at the positive electrode.

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

2 Select Boundary 3 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 1*

It is important to provide appropriate initial values in the model.

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 $cLi$ text field, type `cLi0`.

4 In the *phis* text field, type `Eeq`.

*Initial Values 2*

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

2 Select Domain 1 only.

3 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

4 In the *cLi* text field, type `cLi0`.

### TRANSPORT OF DILUTED SPECIES IN POROUS MEDIA (TDS)

Set up the physics in the porous media transport interface. Mass transport of oxygen in the positive porous electrode is by diffusion only. Quadratic elements are used for oxygen concentration. Also, provide a concentration boundary condition at the positive electrode.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Transport of Diluted Species in Porous Media (tds)**.

2 Select Domain 2 only.

3 In the **Settings** window for **Transport of Diluted Species in Porous Media**, locate the **Transport Mechanisms** section.

4 Clear the **Convection** check box.

5 Click to expand the **Discretization** section. From the **Concentration** list, choose **Quadratic**.

*Fluid 1*

1 In the **Model Builder** window, expand the **Porous Medium 1** node, then click **Fluid 1**.

2 In the **Settings** window for **Fluid**, locate the **Diffusion** section.

3 In the $D_{\mathrm{F,cO2}}$ text field, type `DO2`.

4 From the **Effective diffusivity model** list, choose **Bruggeman model**.

*Porous Matrix 1*

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

2 In the **Settings** window for **Porous Matrix**, locate the **Matrix Properties** section.

3 From the $\varepsilon_p$ list, choose **User defined**. In the associated text field, type `liion.epsl`.

*Concentration 1*

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

2 Select Boundary 3 only.

3 In the **Settings** window for **Concentration**, locate the **Concentration** section.

4 Select the **Species cO2** check box.

5 In the $c_{0,cO2}$ text field, type `c020`.

*Initial Values 1*

Specify an initial value for oxygen concentration.

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 $cO2$ text field, type `c020`.

*Porous Electrode Coupling 1*

Add porous electrode coupling feature to model the consumption of oxygen due to the electrochemical reaction.

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

2 Select Domain 2 only.

*Reaction Coefficients 1*

1 In the **Model Builder** window, expand the **Porous Electrode Coupling 1** node, then click **Reaction Coefficients 1**.

2 In the **Settings** window for **Reaction Coefficients**, locate the **Model Inputs** section.

3 From the $i_v$ list, choose **Local current source, Porous Electrode Reaction 1 (liion/pce1/per1)**.

4 Locate the **Stoichiometric Coefficients** section. In the $n$ text field, type `n`.

5 In the $\nu_{cO2}$ text field, type `-1`.

### DOMAIN ODES AND DAES: CONCENTRATION OF LI2O2

Set up the physics to model the change in concentration of the reaction product (Li2O2) in the solution phase of the positive electrode, by specifying the appropriate source term. Lagrange (Quadratic) elements are used for concentration of the reaction product.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Domain ODEs and DAEs (dode)**.

2 In the **Settings** window for **Domain ODEs and DAEs**, type `Domain ODEs and DAEs: Concentration of Li2O2` in the **Label** text field.

3 Select Domain 2 only.

4 Click to expand the **Discretization** section. From the **Shape function type** list, choose **Lagrange**.

*Distributed ODE 1*

1 In the **Model Builder** window, under **Component 1 (comp1)>**
**Domain ODEs and DAEs: Concentration of Li2O2 (dode)** click **Distributed ODE 1**.

2 In the **Settings** window for **Distributed ODE**, locate the **Source Term** section.

3 In the *f* text field, type `((-liion.ivtot*1)/(2*F_const))*(cLi2O2<cmaxLi2O2)`.

## 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 `T`.

## MESH 1

Select a finer mesh for this model.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Mesh 1**.

2 In the **Settings** window for **Mesh**, locate the **Physics-Controlled Mesh** section.

3 From the **Element size** list, choose **Finer**.

4 Click **Build All**.

## STUDY 1

Set up a parametric study for a range of discharge current densities.

*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 |
|---|---|---|
| a (Used in parametric sweep) | 1 2 4 10 | |

*Step 1: Time Dependent*

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

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

3 In the **Output times** text field, type `0 1e7`.

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

5 In the **Relative tolerance** text field, type `1e-4`.

*Solution 1 (sol1)*

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

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

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

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

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

Store only every 3rd time step. This reduces the size of the stored solution and the size of model file.

5 In the **Store every Nth step** text field, type `3`.

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.EndTerminal(comp1.phis)< 2.5` | True (>=1) | √ | `Stop expression 1` |

10 Locate the **Output at Stop** section. Clear the **Add warning** check box.

11 In the **Model Builder** window, click **Study 1**.

12 In the **Settings** window for **Study**, locate the **Study Settings** section.

13 Clear the **Generate default plots** check box.

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

## RESULTS

*Cell Voltages for different iapp*

First plot the cell voltage for the different discharge current densities (see Figure 2).

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 Voltages for different iapp` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/ Parametric Solutions 1 (sol2)**.

*Point Graph 1*

1 Right-click **Cell Voltages for different iapp** and choose **Point Graph**.

2 Select Boundary 3 only.

3 In the **Settings** window for **Point Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)> Lithium-Ion Battery>phis - Electric potential - V**.

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

5 Click **Replace Expression** in the upper-right corner of the **x-Axis Data** section. From the menu, choose **Component 1 (comp1)>Definitions>Variables>capacity - Specific capacity of cell - C/kg**.

6 Click to expand the **Legends** section. Select the **Show legends** check box.

7 From the **Legends** list, choose **Evaluated**.

8 In the **Legend** text field, type `eval(-i_app,mA/cm^2) mA/cm^2`.

*Cell Voltages for different iapp*

1 In the **Model Builder** window, click **Cell Voltages for different iapp**.

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

3 Select the **x-axis label** check box. In the associated text field, type `Specific capacity of cell (mAh/g)`.

4 Select the **y-axis label** check box. In the associated text field, type `Cell Voltage (V)`.

5 Click to expand the **Title** section. From the **Title type** list, choose **Manual**.

6 In the **Title** text area, type `Cell Voltage`.

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

8 In the **Cell Voltages for different iapp** toolbar, click **Plot**.

*Oxygen conc in positive electrode, iapp = 0.1 mA/cm2*

Next, plot the oxygen concentration in the positive electrode for a low and high value of the discharge current density (see Figure 3 and Figure 4).

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

2 In the **Settings** window for **1D Plot Group**, type `Oxygen conc in positive electrode, iapp = 0.1mA/cm2` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/ Parametric Solutions 1 (sol2)**.

4 From the **Parameter selection (a)** list, choose **From list**.

5 In the **Parameter values (a)** list, select **2**.

*Line Graph 1*

1 Right-click **Oxygen conc in positive electrode, iapp = 0.1mA/cm2** and choose **Line Graph**.

2 Select Domain 2 only.

3 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)> Transport of Diluted Species in Porous Media>Species c02>c02 - Concentration - mol/m³**.

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

5 In the **Expression** text field, type `x/(Lsep+Lpos)`.

6 Select the **Description** check box. In the associated text field, type `Dimensionless thickness of positive electrode`.

*Oxygen conc in positive electrode, iapp = 0.1mA/cm2*

1 In the **Model Builder** window, click **Oxygen conc in positive electrode, iapp = 0.1mA/cm2**.

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

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

4 In the **Title** text area, type `Oxygen concentration in positive electrode`.

5 In the **Oxygen conc in positive electrode, iapp = 0.1mA/cm2** toolbar, click **Plot**.

6 Right-click **Oxygen conc in positive electrode, iapp = 0.1mA/cm2** and choose **Duplicate**.

*Oxygen conc in positive electrode, iapp = 0.5mA/cm2*

1 In the **Model Builder** window, under **Results** click **Oxygen conc in positive electrode, iapp = 0.1mA/cm2.1**.

2 In the **Settings** window for **1D Plot Group**, type `Oxygen conc in positive electrode, iapp = 0.5mA/cm2` in the **Label** text field.

3 Locate the **Data** section. In the **Parameter values (a)** list, select **10**.

4 In the **Oxygen conc in positive electrode, iapp = 0.5mA/cm2** toolbar, click **Plot**.

*Volume fraction of Li2O2 in positive electrode, iapp = 0.1mA/cm2*

Plot the volume fraction of Li2O2 in the positive electrode for a low and high value of the discharge current density (see Figure 5 and Figure 6), as follows.

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

2 In the **Settings** window for **1D Plot Group**, type `Volume fraction of Li2O2 in positive electrode, iapp = 0.1mA/cm2` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/ Parametric Solutions 1 (sol2)**.

4 From the **Parameter selection (a)** list, choose **From list**.

5 In the **Parameter values (a)** list, select **2**.

6 From the **Time selection** list, choose **Interpolated**.

7 In the **Times (s)** text field, type `1 2e5 5e5 1e6 1.15e6`.

*Line Graph 1*

1 Right-click **Volume fraction of Li2O2 in positive electrode, iapp = 0.1mA/cm2** and choose **Line Graph**.

2 Select Domain 2 only.

3 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Definitions> Variables>epsilonLi2O2 - Volume fraction of Li2O2 - 1**.

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

5 In the **Expression** text field, type `x/(Lsep+Lpos)`.

6 Select the **Description** check box. In the associated text field, type `Dimensionless thickness of positive electrode`.

*Volume fraction of Li2O2 in positive electrode, iapp = 0.1mA/cm2*

1 In the **Model Builder** window, click **Volume fraction of Li2O2 in positive electrode, iapp = 0.1mA/cm2**.

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

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

4 In the **Title** text area, type `Volume fraction of Li2O2 in positive electrode`.

5 Locate the **Axis** section. Select the **Manual axis limits** check box.

6 In the **y maximum** text field, type `0.6`.

7 In the **Volume fraction of Li2O2 in positive electrode, iapp = 0.1mA/cm2** toolbar, click **Plot**.

8 Right-click **Volume fraction of Li2O2 in positive electrode, iapp = 0.1mA/cm2** and choose **Duplicate**.

*Volume fraction of Li2O2 in positive electrode, iapp = 0.5mA/cm2*

1 In the **Model Builder** window, under **Results** click **Volume fraction of Li2O2 in positive electrode, iapp = 0.1mA/cm2.1**.

2 In the **Settings** window for **1D Plot Group**, type `Volume fraction of Li2O2 in positive electrode, iapp = 0.5mA/cm2` in the **Label** text field.

3 Locate the **Data** section. In the **Parameter values (a)** list, select **10**.

4 In the **Times (s)** text field, type `1 5e3 2e4 4e4`.

5 In the **Volume fraction of Li2O2 in positive electrode, iapp = 0.5mA/cm2** toolbar, click **Plot**.

*Porosity of positive electrode, iapp = 0.1mA/cm2*

Plot the porosity in the positive electrode for a low and high value of the discharge current density (see Figure 7 and Figure 8), as follows.

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

2 In the **Settings** window for **1D Plot Group**, type `Porosity of positive electrode, iapp = 0.1mA/cm2` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/ Parametric Solutions 1 (sol2)**.

4 From the **Parameter selection (a)** list, choose **From list**.

5 In the **Parameter values (a)** list, select **2**.

6 From the **Time selection** list, choose **Interpolated**.

7 In the **Times (s)** text field, type `1 2e5 5e5 1e6 1.15e6`.

*Line Graph 1*

1 Right-click **Porosity of positive electrode, iapp = 0.1mA/cm2** and choose **Line Graph**.

2 Select Domain 2 only.

3 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

4 In the **Expression** text field, type `liion.epsl`.

5 Select the **Description** check box. In the associated text field, type `Porosity`.

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

7 In the **Expression** text field, type `x/(Lsep+Lpos)`.

8 Select the **Description** check box. In the associated text field, type `Dimensionless thickness of positive electrode`.

*Porosity of positive electrode, iapp = 0.1mA/cm2*

1 In the **Model Builder** window, click **Porosity of positive electrode, iapp = 0.1mA/cm2**.

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

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

4 In the **Title** text area, type `Porosity of positive electrode`.

5 Locate the **Axis** section. Select the **Manual axis limits** check box.

6 In the **y minimum** text field, type `0.15`.

7 In the **y maximum** text field, type `0.75`.

8 In the **Porosity of positive electrode, iapp = 0.1mA/cm2** toolbar, click **Plot**.

9 Right-click **Porosity of positive electrode, iapp = 0.1mA/cm2** and choose **Duplicate**.

*Porosity of positive electrode, iapp = 0.5mA/cm2*

1 In the **Model Builder** window, under **Results** click **Porosity of positive electrode, iapp = 0.1mA/cm2.1**.

2 In the **Settings** window for **1D Plot Group**, type `Porosity of positive electrode, iapp = 0.5mA/cm2` in the **Label** text field.

3 Locate the **Data** section. In the **Parameter values (a)** list, select **10**.

4 In the **Times (s)** text field, type `1 5e3 2e4 4e4`.

5 In the **Porosity of positive electrode, iapp = 0.5mA/cm2** toolbar, click **Plot**.