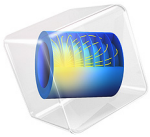

Parasitic Reactions in an Electrochemical Capacitor

Introduction

This model demonstrates how to set up side reactions in an electrochemical supercapacitor using the Tertiary Current Distribution, Nernst–Planck (tcd) interface.

The 1D isothermal model includes the following processes:

- Electronic current conduction in the electrodes
- Ionic charge transport in the porous electrodes and separator
- Double layer capacitance in the porous electrodes
- Side reactions involving hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) for an aqueous electrolyte

The model is based on the theoretical framework of Newman (Ref. 1) and White (Ref. 2). In the model presented, the effect of the parasitic reactions in an aqueous electrolyte-based supercapacitor on the performance during charge discharge behavior is studied.

See also the Electrochemical Capacitor with Porous Electrodes tutorial for an introduction to electrochemical capacitor modeling using the Tertiary Current Distribution interface.

Model Definition

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

- Two porous electrode (right and left): 50 μm
- Separator (flooded with electrolyte): 25 μm

DOMAIN CONDITIONS

The model solves for the potentials in the electrode and aqueous electrolyte phases, in combination with four concentration dependent variables for the cation, the anion and the dissolved concentrations of hydrogen and oxygen.

Due to the aqueous electrolyte, proton and hydroxide transport are also included in the model. Using two algebraic equations: electroneutrality and the water-autoprotolysis to be in equilibrium, the proton and hydroxide concentrations do not need to be solved for as dependent variables.

The electric potential in the electron conducting phase, ϕ_s, is calculated using a charge balance based on Ohm's law. The migrative and diffusive charge and species transport in the electrolyte is modeled using the Nernst–Planck equations.

The double layer charging is defined as a source term in the porous electrodes based on the time derivative of the potential jump over the double layer according to

$$i_{v,\,\mathrm{dl}} = a_{v,\,\mathrm{dl}} C_{\mathrm{dl}} \frac{\mathrm{d}(\phi_s - \phi_l)}{\mathrm{d}t} \tag{1}$$

where $a_{v,\mathrm{dl}}$ ($\mathrm{m}^2/\mathrm{m}^3$) is the active specific surface area for double layer charging, and C_{dl} is the double layer capacitance (F/m^2).

Due to the aqueous electrolyte, oxygen and hydrogen may start evolving in the electrodes. In the positive porous electrode, oxygen evolution, or reduction, occurs according to

$$\mathrm{O_2} + 4\mathrm{H^+} + 4e^- \leftrightarrow 2\mathrm{H_2O} \tag{2}$$

In the negative porous electrode, hydrogen evolution, or oxidation, occurs according to

$$2\mathrm{H^+} + 2e^- \leftrightarrow \mathrm{H_2} \tag{3}$$

The porous electrode reactions are modeled using concentration-dependent Butler–Volmer reactions.

BOUNDARY CONDITIONS

For the electronic current balance, a potential of 0 V is set on the left electrode's current collector/feeder boundary.

At the right electrode current collector/feeder, an event-based charge-discharge condition is used. First the capacitor is charged at 100 A until a voltage of 2 V is reached, then the capacitor rests for 1 h, followed by a discharge at 100 A until a voltage of 0.5 V is reached. The cycle is then repeated.

At the separator-negative electrode boundary, it is assumed that the electrode potential is so low that oxygen, produced at the positive electrode and diffusing over the separator, will be immediately reduced at this point. Similarly, at the separator-positive electrode boundary, it is assumed that any hydrogen reaching this point will be immediately reduced.

The above conditions are modeled by setting the respective hydrogen or oxygen concentration to 0 at the electrode-separator boundaries, and by adding the corresponding electrode current density (based on the species flux and Faraday's law) to the charge balance equations. This is achieved using an Internal Electrode Surface boundary node.

Results and Discussion

Figure 1 shows the current-voltage response versus time for a 5000 simulation. Each charge pulse is followed by 1 h during which the voltage relaxes due to the parasitic oxygen reduction and hydrogen oxidation at the electrode-separator boundaries.

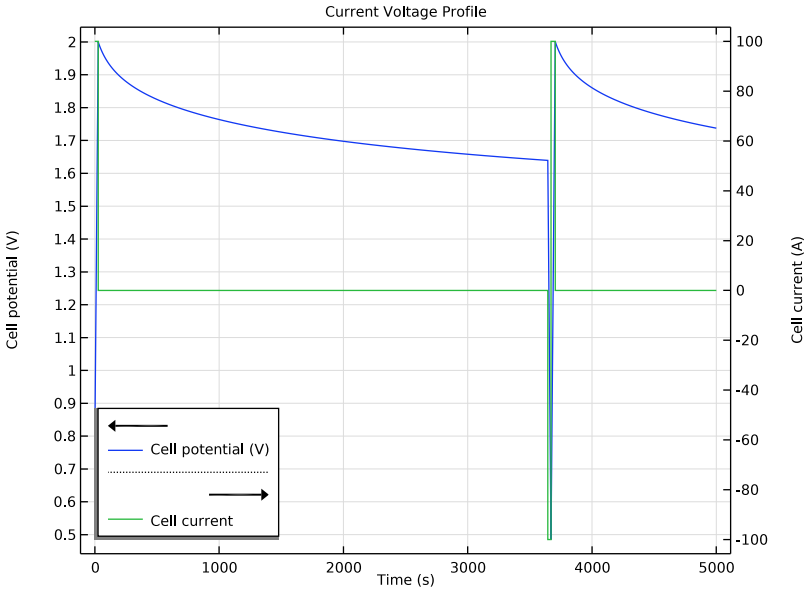

Figure 1: Voltage and current profiles for the capacitor.

Figure 2 shows the maximum activities (the concentration divided by the respective solubility limit) in the cell for the oxygen and hydrogen species versus time. The activities increase during the charge pulses, and relax linearly versus time during the rest period.

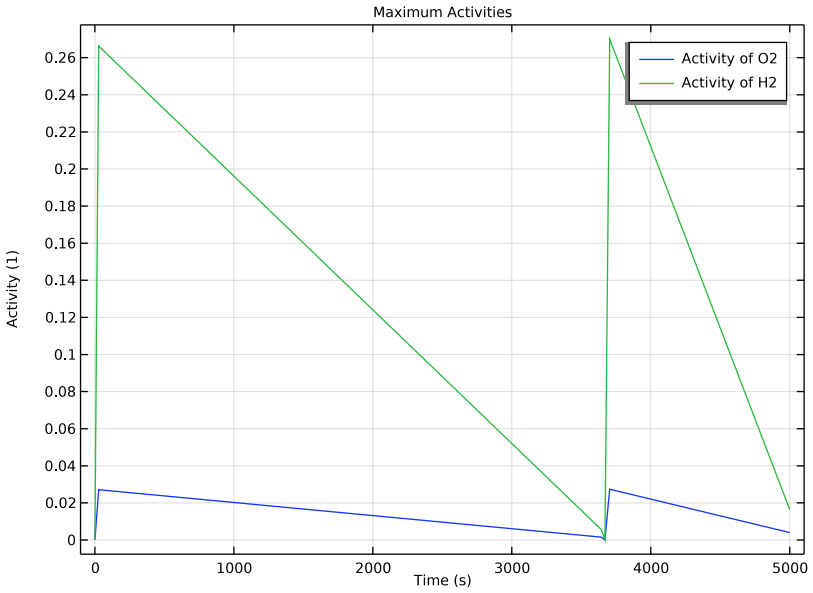

Figure 2: Maximum cell activity for O_2 and H_2 versus time.

Figure 3, finally, shows oxygen and hydrogen concentrations in the cell at the end of a charge period. The maximum values are found at the separator-current collector boundaries.

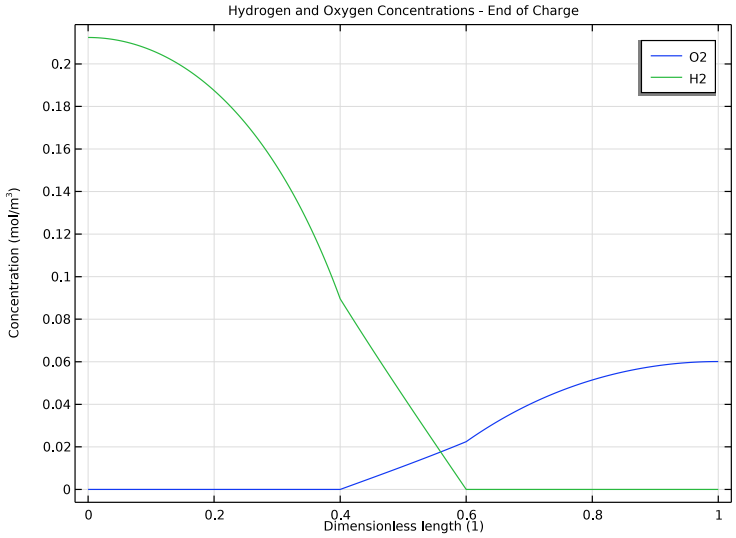

Figure 3: Concentrations of O_2 and H_2 at the end of charge.

References

1. M.B. Pillay and J. Newman, "The Influence of Side Reactions on the Performance of Electrochemical Double-Layer Capacitance," *J. Electrochem. Soc.*, vol. 143, no. 6, pp. 1806–1814, 1996.

2. C.Lin, J.A. Ritter, B.N. Popov, and R.E. White, "A Mathematical Model of an Electrochemical Capacitor with Double Layer and Faradaic Processes," *J. Electrochem. Soc.*, vol. 146, no. 9, pp. 3168–3175, 1999.

Application Library path: `Battery_Design_Module/Electrochemical_Capacitors/electrochemical_capacitor_side_reactions`

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>Tertiary Current Distribution, Nernst-Planck>Tertiary, Water-Based with Electroneutrality (tcd)**.

3 Click **Add**.

4 Click **Study**.

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

6 Click **Done**.

GLOBAL DEFINITIONS

Parameters : Electrochemical Cell

Import the parameter file for the electrochemical cell, the load profile and for the parasitic electrode reactions.

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 `electrochemical_capacitor_side_reactions_electrochemical_cell.txt`.

5 In the **Label** text field, type `Parameters : Electrochemical Cell`.

Parameters : Load Profile

1 In the **Home** toolbar, click **Parameters** and choose **Add>Parameters**.

2 In the **Settings** window for **Parameters**, type `Parameters : Load Profile` in the **Label** text field.

3 Locate the **Parameters** section. Click **Load from File**.

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

Parameters : Electrode Reactions

1 In the **Home** toolbar, click **Parameters** and choose **Add>Parameters**.

2 In the **Settings** window for **Parameters**, type `Parameters : Electrode Reactions` in the **Label** text field.

3 Locate the **Parameters** section. Click **Load from File**.

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

GEOMETRY 1

Interval 1 (i1)

1 In the **Model Builder** window, expand the **Component 1 (comp1)>Geometry 1** node.

2 Right-click **Geometry 1** and choose **Interval**.

GEOMETRY 1

Interval 1 (i1)

1 In the **Model Builder** window, expand the **Component 1 (comp1)>Geometry 1> Interval 1 (i1)** node, then click **Interval 1 (i1)**.

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_elec
L_sep
L_elec

Form Union (fin)

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

TERTIARY CURRENT DISTRIBUTION, NERNST-PLANCK (TCD)

Add the dependent variables for the concentration of the different electroactive species.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Tertiary Current Distribution, Nernst-Planck (tcd)**.

2 In the **Settings** window for **Tertiary Current Distribution, Nernst-Planck**, click to expand the **Dependent Variables** section.

3 In the **Number of species** text field, type 4.

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

cCat
cAn

cO2
cH2

Species Charges 1

Define the migration parameters in the electrolyte.

1. In the **Model Builder** window, under **Component 1 (comp1)>Tertiary Current Distribution, Nernst-Planck (tcd)** click **Species Charges 1**.
2. In the **Settings** window for **Species Charges**, locate the **Charge** section.
3. In the z_{cCat} text field, type `1`.
4. In the z_{cAn} text field, type `-1`.

Electrolyte 1

Define the diffusion parameters in the electrolyte.

1. In the **Model Builder** window, click **Electrolyte 1**.
2. In the **Settings** window for **Electrolyte**, locate the **Diffusion** section.
3. In the D_{cCat} text field, type `D`.
4. In the D_{cAn} text field, type `D`.
5. In the D_{cO2} text field, type `D_O2`.
6. In the D_{cH2} text field, type `D_H2`.

Initial Values - H2 side

Set the initial values for the different domains of the electrochemical cell.

1. In the **Model Builder** window, under **Component 1 (comp1)>Tertiary Current Distribution, Nernst-Planck (tcd)** click **Initial Values 1**.
2. In the **Settings** window for **Initial Values**, type `Initial Values - H2 side` in the **Label** text field.
3. Locate the **Initial Values** section. In the *cCat* text field, type `c_bulk`.
4. In the *cAn* text field, type `c_bulk`.
5. In the *cH2* text field, type `cH2_init`.

Initial Values - O2 side

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. Click **Paste Selection**.
4. In the **Paste Selection** dialog box, type `3` in the **Selection** text field.

5 Click **OK**.

6 In the **Settings** window for **Initial Values**, type `Initial Values - O2 side` in the **Label** text field.

7 Locate the **Initial Values** section. In the *cCat* text field, type `c_bulk`.

8 In the *cAn* text field, type `c_bulk`.

9 In the *cO2* text field, type `cO2_init`.

10 In the *phis* text field, type `E_cell_init`.

Initial Values - Separator

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

2 In the **Settings** window for **Initial Values**, type `Initial Values - Separator` in the **Label** text field.

3 Locate the **Domain Selection** section. Click **Paste Selection**.

4 In the **Paste Selection** dialog box, type `2` in the **Selection** text field.

5 Click **OK**.

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

7 In the *cCat* text field, type `c_bulk`.

8 In the *cAn* text field, type `c_bulk`.

9 In the *cO2* text field, type `cO2_init*(x-L_elec)/L_sep`.

10 In the *cH2* text field, type `cH2_init*(L_elec+L_sep-x)/L_sep`.

11 In the *phis* text field, type `E_cell_init`.

Porous Electrode - H2 side

Set the properties of the porous electrode and the electrode reactions at the respective electrode domains.

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

2 In the **Settings** window for **Porous Electrode**, type `Porous Electrode - H2 side` in the **Label** text field.

3 Locate the **Domain Selection** section. Click **Paste Selection**.

4 In the **Paste Selection** dialog box, type `1` in the **Selection** text field.

5 Click **OK**.

6 In the **Settings** window for **Porous Electrode**, locate the **Diffusion** section.

7 In the D_{cCat} text field, type `D`.

8 In the D_{cAn} text field, type `D`.

9 In the D_{cO2} text field, type `D_O2`.

10 In the D_{cH2} text field, type `D_H2`.

11 Locate the **Electrode Current Conduction** section. From the σ_s list, choose **User defined**. In the associated text field, type `sigma_s`.

12 Locate the **Porous Matrix Properties** section. In the ε_s text field, type `1-eps_el`.

13 In the ε_l text field, type `eps_el`.

Porous Electrode Reaction - HER

1 In the **Model Builder** window, under **Component 1 (comp1)>Tertiary Current Distribution, Nernst-Planck (tcd)>Porous Electrode - H2 side** click **Porous Electrode Reaction 1**.

2 In the **Settings** window for **Porous Electrode Reaction**, type `Porous Electrode Reaction - HER` in the **Label** text field.

3 Locate the **Stoichiometric Coefficients** section. In the ν_{cH2} text field, type `1`.

4 In the n text field, type `2`.

5 Locate the **Equilibrium Potential** section. In the $E_{eq,ref}(T)$ text field, type `Eeq_ref_H2`.

6 Locate the **Electrode Kinetics** section. In the $i_{0,ref}(T)$ text field, type `i0_ref_H2`.

7 Locate the **Active Specific Surface Area** section. In the a_v text field, type `Av`.

Porous Electrode - H2 side

In the **Model Builder** window, click **Porous Electrode - H2 side**.

Porous Matrix Double Layer Capacitance 1

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

2 In the **Settings** window for **Porous Matrix Double Layer Capacitance**, locate the **Porous Matrix Double Layer Capacitance** section.

3 In the C_{dl} text field, type `aC`.

4 In the $a_{v,dl}$ text field, type `Av`.

5 Locate the **Stoichiometric Coefficients** section. In the ν_{cCat} text field, type `-0.5`.

6 In the ν_{cAn} text field, type `0.5`.

Porous Electrode - H2 side

Right-click **Porous Electrode - H2 side** and choose **Duplicate**.

Porous Electrode - O2 side

1 In the **Model Builder** window, under **Component 1 (comp1)>Tertiary Current Distribution, Nernst-Planck (tcd)** click **Porous Electrode - H2 side 1**.

2 In the **Settings** window for **Porous Electrode**, type `Porous Electrode - O2 side` in the **Label** text field.

3 Locate the **Domain Selection** section. Click **Clear Selection**.

4 Click **Paste Selection**.

5 In the **Paste Selection** dialog box, type `3` in the **Selection** text field.

6 Click **OK**.

Porous Electrode Reaction - OER

1 In the **Model Builder** window, expand the **Porous Electrode - O2 side** node, then click **Porous Electrode Reaction - HER**.

2 In the **Settings** window for **Porous Electrode Reaction**, type `Porous Electrode Reaction - OER` in the **Label** text field.

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

4 In the ν_{cO2} text field, type `-1`.

5 In the ν_{cH2} text field, type `0`.

6 Locate the **Equilibrium Potential** section. In the $E_{eq,ref}(T)$ text field, type `Eeq_ref_O2`.

7 Locate the **Electrode Kinetics** section. In the $i_{0,ref}(T)$ text field, type `i0_ref_O2`.

Define the recombination reaction on the internal boundaries.

Internal Electrode Surface -ORR

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

2 In the **Settings** window for **Internal Electrode Surface**, type `Internal Electrode Surface -ORR` in the **Label** text field.

3 Locate the **Boundary Selection** section. Click **Paste Selection**.

4 In the **Paste Selection** dialog box, type `2` in the **Selection** text field.

5 Click **OK**.

Electrode Reaction 1

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

2 In the **Settings** window for **Electrode Reaction**, locate the **Stoichiometric Coefficients** section.

3 In the n text field, type `4`.

4 In the ν_{cO2} text field, type `-1`.

5 Locate the **Equilibrium Potential** section. From the E_{eq} list, choose **User defined**. Locate the **Electrode Kinetics** section. From the **Kinetics expression type** list, choose **Fast irreversible electrode reaction**.

6 From the c_{lim} list, choose **cO2**.

Internal Electrode Surface -ORR

In the **Model Builder** window, right-click **Internal Electrode Surface -ORR** and choose **Duplicate**.

Internal Electrode Surface -HOR

1 In the **Model Builder** window, click **Internal Electrode Surface -ORR 1**.

2 In the **Settings** window for **Internal Electrode Surface**, locate the **Boundary Selection** section.

3 In the list, select **2**.

4 Click — **Remove from Selection**.

5 Select Boundary 3 only.

6 In the **Label** text field, type `Internal Electrode Surface -HOR`.

Electrode Reaction 1

1 In the **Model Builder** window, expand the **Internal Electrode Surface -HOR** node, then click **Electrode Reaction 1**.

2 In the **Settings** window for **Electrode Reaction**, locate the **Stoichiometric Coefficients** section.

3 In the n text field, type `2`.

4 In the ν_{cO2} text field, type `0`.

5 In the ν_{cH2} text field, type `1`.

6 Locate the **Electrode Kinetics** section. From the c_{lim} list, choose **cH2**.

Electric Ground 1

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

2 In the **Settings** window for **Electric Ground**, locate the **Boundary Selection** section.

3 Click **Paste Selection**.

4 In the **Paste Selection** dialog box, type `1` in the **Selection** text field.

5 Click **OK**.

Charge-Discharge Cycling 1

Set up the load cycle using the charge-discharge cycle boundary condition.

1 In the **Physics** toolbar, click **Boundaries** and choose **Charge-Discharge Cycling**.

2 In the **Settings** window for **Charge-Discharge Cycling**, locate the **Boundary Selection** section.

3 Click **Paste Selection**.

4 In the **Paste Selection** dialog box, type 4 in the **Selection** text field.

5 Click **OK**.

6 In the **Settings** window for **Charge-Discharge Cycling**, locate the **Discharge Settings** section.

7 In the I_{dch} text field, type `-I_app`.

8 In the V_{min} text field, type `V_min`.

9 Locate the **Charge Settings** section. In the I_{ch} text field, type `I_app`.

10 In the V_{max} text field, type `V_max`.

11 Select the **Include rest period** check box.

12 In the $t_{\mathrm{rest,ch}}$ text field, type `t_rest`.

13 Click to expand the **Start Mode** section. From the **Start with** list, choose **Charge first**.

14 In the $\phi_{\mathrm{s,bnd,init}}$ text field, type `E_cell_init`.

DEFINITIONS

Add probes using the definitions node in the model builder for the activities of H2 and O2, and the cell potential.

Domain Probe 1 (dom1)

1 In the **Definitions** toolbar, click **Probes** and choose **Domain Probe**.

2 In the **Settings** window for **Domain Probe**, type `aH2` in the **Variable name** text field.

3 Locate the **Probe Type** section. From the **Type** list, choose **Maximum**.

4 Locate the **Expression** section. In the **Expression** text field, type `comp1.cH2/cH2_sol`.

5 Select the **Description** check box. In the associated text field, type `aH2`.

Domain Probe 1 (aH2)

Right-click **Domain Probe 1 (aH2)** and choose **Duplicate**.

Domain Probe 2 (dom2)

1 In the **Model Builder** window, under **Component 1 (comp1)>Definitions** click **Domain Probe 2 (dom2)**.

2 In the **Settings** window for **Domain Probe**, type `aO2` in the **Variable name** text field.

3 Locate the **Expression** section. In the **Expression** text field, type `comp1.cO2/cO2_sol`.

4 In the **Description** text field, type `a02`.

Global Variable Probe 1 (var1)

1 In the **Definitions** toolbar, click  **Probes** and choose **Global Variable Probe**.

2 In the **Settings** window for **Global Variable Probe**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)> Tertiary Current Distribution, Nernst-Planck>Charge-Discharge Cycling 1>tcd.cdc1.phis0 - Cell potential - V**.

3 In the **Variable name** text field, type `E_cell`.

Maximum 1 (maxop1)

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

2 In the **Settings** window for **Maximum**, locate the **Source Selection** section.

3 From the **Selection** list, choose **All domains**.

GLOBAL DEFINITIONS

Set the temperature for the model using common model inputs.

Default Model Inputs

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

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Mesh 1** and choose **Build All**.

2 Click the  **Zoom Extents** button in the **Graphics** toolbar.

STUDY 1 : CC CHARGE WITH REST PERIOD

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

2 In the **Settings** window for **Study**, type `Study 1 : CC Charge with Rest Period` in the **Label** text field.

3 Locate the **Study Settings** section. Clear the **Generate default plots** check box.

Step 1: Time Dependent

1 In the **Model Builder** window, expand the **Study 1 : CC Charge with Rest Period** node, then 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 5000`.

Solution 1 (sol1)

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

2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node.

3 Right-click **Study 1 : CC Charge with Rest Period>Solver Configurations>Solution 1 (sol1)> Time-Dependent Solver 1** and choose **Compute**.

RESULTS

Plot the current voltage profile for the capacitor.

Current Voltage Profile

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

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

3 Click to expand the **Title** section. From the **Title type** list, choose **Label**.

4 Locate the **Legend** section. From the **Position** list, choose **Lower left**.

Cell Potential

1 Right-click **Current Voltage Profile** and choose **Table Graph**.

2 In the **Settings** window for **Table Graph**, type `Cell Potential` in the **Label** text field.

3 Locate the **Data** section. From the **Plot columns** list, choose **Manual**.

4 In the **Columns** list, select **Cell potential (V)**.

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

6 In the **Current Voltage Profile** toolbar, click **Plot**.

Cell Current

1 In the **Model Builder** window, right-click **Current Voltage Profile** and choose **Global**.

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)> Tertiary Current Distribution, Nernst-Planck>Charge-Discharge Cycling 1>tcd.cdc1.Icell - Cell current - A**.

3 In the **Label** text field, type `Cell Current`.

Current Voltage Profile

1 In the **Model Builder** window, click **Current Voltage Profile**.

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

3 Select the **Two y-axes** check box.

4 In the table, select the **Plot on secondary y-axis** check box for **Cell Current**.

5 In the **Current Voltage Profile** toolbar, click **Plot**.

6 Click the **Zoom Extents** button in the **Graphics** toolbar.

Maximum Activities

Plot the maximum and minimum activities for O2 and H2.

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

2 In the **Settings** window for **1D Plot Group**, type `Maximum Activities` in the **Label** text field.

3 Click to expand the **Title** section. From the **Title type** list, choose **Label**.

4 Locate the **Plot Settings** section.

5 Select the **y-axis label** check box. In the associated text field, type `Activity (1)`.

Activity of O2

1 Right-click **Maximum Activities** and choose **Global**.

2 In the **Settings** window for **Global**, type `Activity of O2` in the **Label** text field.

3 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
`maxop1(cO2/cO2_sol)`	1	`Activity of O2`

4 Right-click **Activity of O2** and choose **Duplicate**.

Activity of H2

1 In the **Model Builder** window, under **Results>Maximum Activities** click **Activity of O2.1**.

2 In the **Settings** window for **Global**, type `Activity of H2` in the **Label** text field.

3 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
`maxop1(cH2/cH2_sol)`	1	`Activity of H2`

4 In the **Maximum Activities** toolbar, click **Plot**.

5 Click the **Zoom Extents** button in the **Graphics** toolbar.

Hydrogen and Oxygen Concentrations - End of Charge

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

2 In the **Settings** window for **1D Plot Group**, type `Hydrogen and Oxygen Concentrations - End of Charge` in the **Label** text field.

3 Locate the **Data** section. From the **Time selection** list, choose **From list**.

4 In the **Times (s)** list, select **27.388**.

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

6 Locate the **Plot Settings** section.

7 Select the **x-axis label** check box. In the associated text field, type `Dimensionless length (1)`.

8 Select the **y-axis label** check box. In the associated text field, type `Concentration (mol/m<sup>3</sup>)`.

Oxygen Concentration

1 Right-click **Hydrogen and Oxygen Concentrations - End of Charge** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, type `Oxygen Concentration` in the **Label** text field.

3 Locate the **Selection** section. From the **Selection** list, choose **All domains**.

4 Locate the **y-Axis Data** section. In the **Expression** text field, type `cO2`.

5 Select the **Description** check box. In the associated text field, type `O2`.

6 In the **Hydrogen and Oxygen Concentrations - End of Charge** toolbar, click **Plot**.

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

8 In the **Expression** text field, type `x/(2*L_elec+L_sep)`.

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

10 Find the **Include** subsection. Clear the **Solution** check box.

11 Select the **Description** check box.

12 In the **Hydrogen and Oxygen Concentrations - End of Charge** toolbar, click **Plot**.

13 Right-click **Oxygen Concentration** and choose **Duplicate**.

Hydrogen Concentration

1 In the **Model Builder** window, expand the **Oxygen Concentration** node, then click **Results> Hydrogen and Oxygen Concentrations - End of Charge>Oxygen Concentration 1**.

2 In the **Settings** window for **Line Graph**, type `Hydrogen Concentration` in the **Label** text field.

3 Locate the **y-Axis Data** section. In the **Expression** text field, type `cH2`.

4 Select the **Description** check box. In the associated text field, type `H2`.

5 In the **Hydrogen and Oxygen Concentrations - End of Charge** toolbar, click  **Plot**.

6 Click the  **Zoom Extents** button in the **Graphics** toolbar.