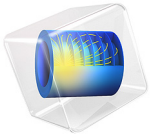

Electrochemical Capacitor with Porous Electrodes

Introduction

This model demonstrates how to set up 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

The model is based on a paper by M.W. Verbrugge (Ref. 1). In the paper, the authors analyze the effect of the microstructure of the porous electrodes on the performance of a supercapacitor with a relatively high specific energy.

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 the binary non-aqueous electrolyte phases, in combination with a concentration dependent variable for one of the ions. The concentration for the other ion is calculated from the condition of electroneutrality.

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 are modeled using the Nernst–Planck equations, assuming electroneutrality.

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).

The effective electrical conductivity in porous electrodes σ_s^{eff}, is defined by taking porosity and tortuosity into account through the expression

$$\sigma_s^{\mathrm{eff}} = \frac{\varepsilon}{\tau}\sigma_s$$

where ε is the porosity parameter and τ is the tortuosity parameter. The effective ionic conductivities in the porous electrodes and the separator are also calculated similarly.

Similarly, the effective diffusion coefficient, D^{eff}, for the electrolyte salt corrects for the porosity and the tortuosity through

$$D^{\mathrm{eff}} = \frac{\varepsilon}{\tau}D$$

The ionic charge balances are modeled according to the electroneutrality condition in the bulk of the binary 1:1 electrolyte (Ref. 1). The mobilities, u_i, of the ionic species under migration are calculated via the Nernst–Einstein relation:

$$u_i = \frac{D_i}{RT}$$

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, either the current density or power is specified. The inner boundaries facing the separator are insulating for electric currents.

For Study 1, current density is calculated by the use of a global equation node. For Study 2, a constant power charging is specified at the right porous electrode boundary. The initial values are specified using the rest potentials. Parametric sweep is used to simulate different values of applied power and resting potential.

EVENTS INTERFACE - CONSTANT CURRENT CHARGE - CONSTANT VOLTAGE DISCHARGE

The Events interface is used to simulate the load cycle comprising CC charge – CV discharge source. The Event Sequence feature is used to set up events for the CC step, the CV step, and the rest period.

Simulations of constant current (CC) charge-constant voltage (CV) discharge are performed in Study 1.

CURRENT AND VOLTAGE PROFILE FOR CC-CHARGE CV-DISCHARGE

The capacitor is charged to 1.8 V at a constant current of 100 A followed by constant voltage for 5 s and a rest stage of 180 s. This procedure is repeated while incrementing the maximum voltage (`V_max`) by 0.2 V until it reaches 2.45 V. Figure 1 shows the current-voltage response for times until the maximum voltage of 2.45 V is reached.

VOLTAGE AND CURRENT PROFILES FOR CC-CHARGE CV-DISCHARGE CYCLE

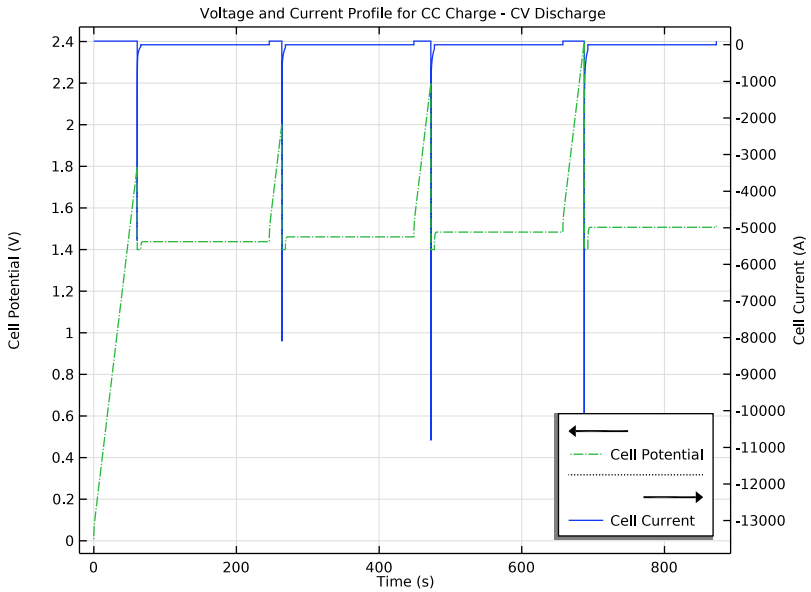

Figure 1: Voltage and current profiles for the events-based load profile.

Figure 2 shows current and voltage profiles overlapped to depict each cycle between constant current charges for incremented maximum voltage values. To achieve the overlapping, filters have been used for plotting the current and voltage profile (see Modeling Instructions).

VOLTAGE AND CURRENT PROFILES FOR CC CHARGING-CV DISCHARGE OVERLAPPED

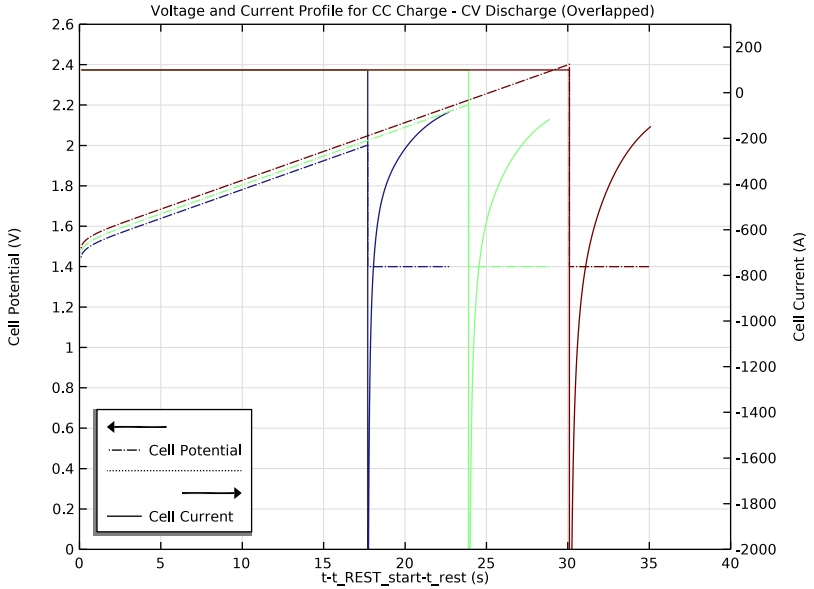

Figure 2: Overlapped current and voltage profiles for the event-based load profile.

STUDY 2: CONSTANT POWER CHARGING

Figure 3 shows the double-layer current for the constant power discharge for the dimensionless length of the electrochemical cell. Figure 4 shows the charge density distribution over the dimensionless length of the electrochemical cell for constant power charge. Figure 3 and Figure 4 can collectively be seen as the indicator for electrode utilization. They show that for a higher cell power, there is a nonuniform charge distribution and poor electrode utilization. This, in turn, can lead to poor capacitor design and underutilization of electrodes despite involving porous structure for more active area.

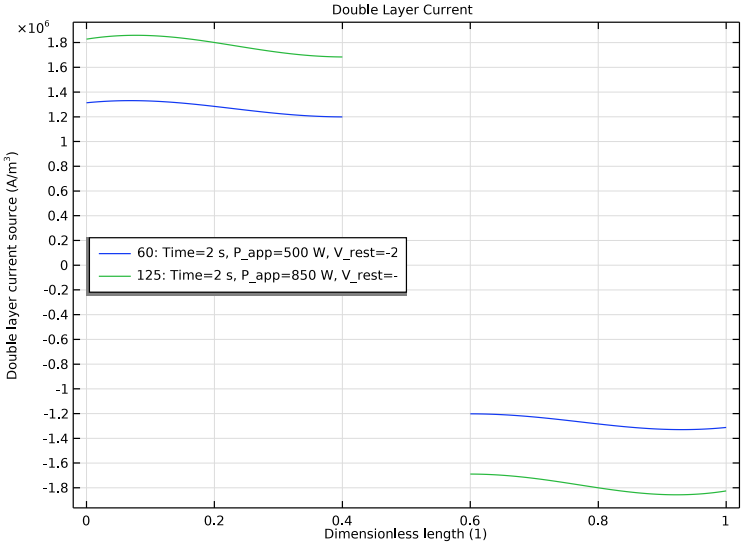

Figure 3: Double layer current source for constant power charging.

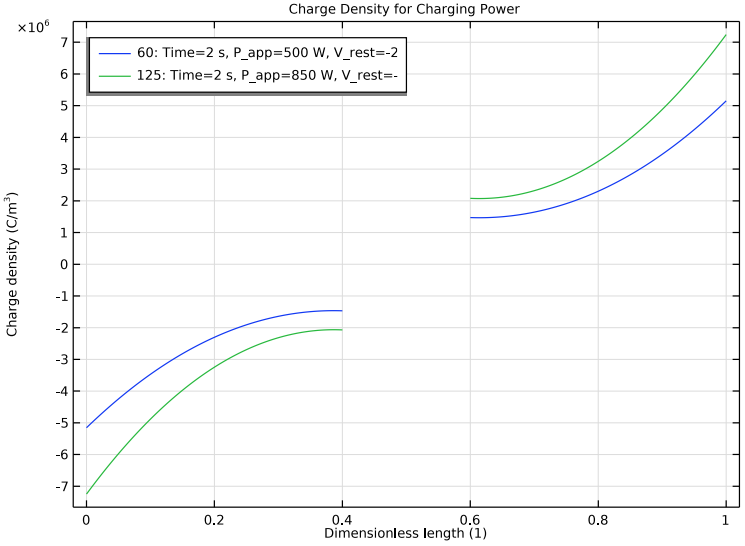

Figure 4: Charge density plotted over the dimensionless length of the cell.

Figure 5 shows the current and voltage profiles for different applied power parameter. For the higher charging power, the voltage change is larger.

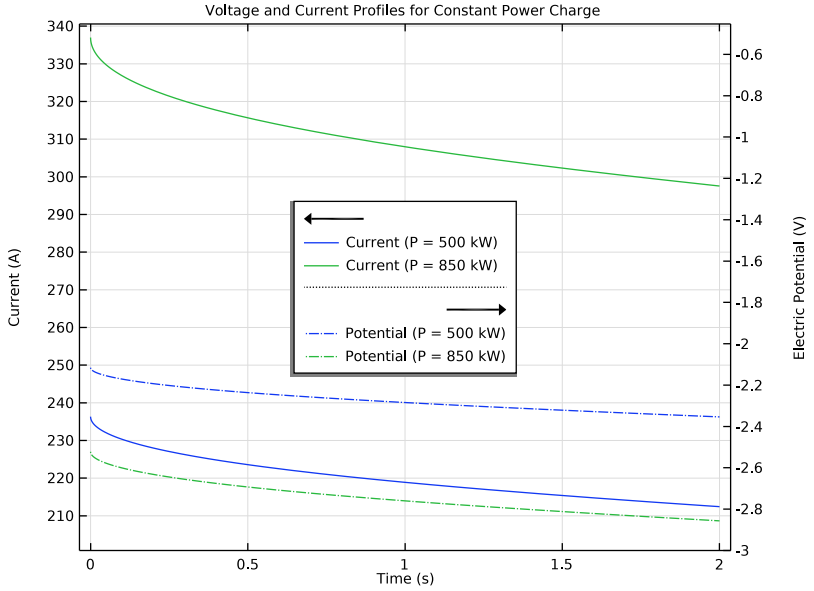

Figure 5: Current and voltage profiles for constant voltage charging.

Notes About the COMSOL Implementation

DEPOSITING-DISSOLVING SPECIES

The charge density for the double layer kinetics can be monitored using the depositing-dissolving species and non-Faradaic reaction nodes. The reaction rate for the non-Faradaic process (capacitor charge discharge) is set proportional to the double layer current inside the porous electrode.

POROUS ELECTRODE AREA AND TORTUOSITY

The area of the porous electrodes parameter used in the model is calculated from the nominal capacitance of 3,500 F as given in Ref. 1. The result reported in Ref. 1 for the constant power can be reproduced by changing the specific area parameter to 27,470 cm^2.

The value for electrode tortuosity is not reported in the reference and is assumed to be unity in the current study. For reproduction of the results for constant power, set the tortuosity 2.3.

Reference

1. M.W. Verbrugge and P. Liu, "Microstructural Analysis and Mathematical Modeling of Electric Double-Layer Supercapacitors", *J. Electrochem. Soc.*, vol. 152, no. 5, pp. D79–D87, 2005.

Application Library path: `Battery_Design_Module/Electrochemical_Capacitors/electrochemical_capacitor_porous_electrodes`

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, 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 electrochemical cell.

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_porous_electrodes_cell_parameters.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**.

To this parameter node, import the file containing the parameters for the different load profiles.

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_porous_electrodes_load_parameters.txt`.

GEOMETRY 1

Interval 1 (i1)

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

2 Right-click **Component 1 (comp1)>Geometry 1** and choose **Interval**.

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

4 In the **Settings** window for **Interval**, locate the **Interval** section.

5 From the **Specify** list, choose **Interval lengths**.

6 In the table, enter the following settings:

Lengths (m)
L_elec
L_sep
L_elec

7 Click **Build All Objects**.

TERTIARY CURRENT DISTRIBUTION, NERNST-PLANCK (TCD)

Species Charges 1

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_{c1} text field, type `1`.

4 In the z_{c2} text field, type `-1`.

Electrolyte 1

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

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

3 In the D_{c1} text field, type `D`.

4 In the D_{c2} text field, type `D`.

Initial Values 1

1 In the **Model Builder** window, click **Initial Values 1**.

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

3 In the $c2$ text field, type `c_bulk`.

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

We will now set up the capacitive porous electrodes in the physics. Start with defining the transport and microstructural properties for these electrodes. Note that we will use only one porous domain node to define both the electrodes. To monitor the charge flux we add a depositing-dissolving species **(c1_q)** to the porous electrode node.

Porous Electrode 1

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

2 Select Domains 1 and 3 only.

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

4 In the D_{c1} text field, type `D`.

5 In the D_{c2} text field, type `D`.

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

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

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

9 Locate the **Effective Transport Parameter Correction** section. From the **Diffusion** list, choose **Tortuosity**.

10 Locate the **Porous Matrix Properties** section. In the τ_l text field, type `tau_electrolyte`.

11 Locate the **Effective Transport Parameter Correction** section. From the **Electrical conductivity** list, choose **Tortuosity**.

12 Locate the **Porous Matrix Properties** section. In the τ_s text field, type `tau_electrode`.

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

14 In the table, enter the following settings:

Species	Density (kg/m^3)	Molar mass (kg/mol)
c1_q	8960	0.06355

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

16 Clear the **Subtract volume change from electrolyte volume fraction** check box.

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 `Cdl`.

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

5 Locate the **Stoichiometric Coefficients** section. In the ν_{c2} text field, type `-0.5`.

Porous Electrode Reaction 1

Since, there is no Faradaic reaction taking place at the porous electrodes, disable the porous electrode reaction.

In the **Model Builder** window, right-click **Porous Electrode Reaction 1** and choose **Disable**.

Porous Electrode 1

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

Non-Faradaic Reactions 1

1 In the **Physics** toolbar, click **Attributes** and choose **Non-Faradaic Reactions**.

2 In the **Settings** window for **Non-Faradaic Reactions**, locate the **Reaction Rate** section.

3 In the **Reaction rate for dissolving-depositing species** table, enter the following settings:

Species	Reaction rate (mol/(m^3*s))
`cl_q`	`tcd.ivdl/F_const`

Separator 1

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

2 Select Domain 2 only.

3 In the **Settings** window for **Separator**, locate the **Diffusion** section.

4 In the D_{c1} text field, type `D`.

5 In the D_{c2} text field, type `D`.

6 Locate the **Porous Matrix Properties** section. In the ε_l text field, type `eps_sep`.

7 Locate the **Effective Transport Parameter Correction** section. From the **Diffusion** list, choose **Tortuosity**.

8 Locate the **Porous Matrix Properties** section. In the τ_l text field, type `tau_sep`.

Electric Ground 1

1 In the **Model Builder** window, expand the **Separator 1** node.

2 Right-click **Tertiary Current Distribution, Nernst-Planck (tcd)** and choose **Electrode> Electric Ground**.

3 Select Boundary 1 only.

Electrode Current Density 1

We use the electrode current density to describe the load profile at the boundary.

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

2 Select Boundary 4 only.

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

4 In the $i_{n,s}$ text field, type `i_app_ch/A_cell`.

DEFINITIONS

Define the integration operator at the boundary 4 to be used in the events interface.

Integration 1 (intop1)

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

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

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

4 Select Boundary 4 only.

5 In the **Operator name** text field, type `right_el`.

COMPONENT 1 (COMP1)

We will use the Events interface to set up the load cycle for the electrochemical cell. The **Event Sequence** feature will be used to configure the three parts of the cycle.

ADD PHYSICS

1 In the **Home** toolbar, click **Add Physics** to open the **Add Physics** window.

2 Go to the **Add Physics** window.

3 In the tree, select **Mathematics>ODE and DAE Interfaces>Events (ev)**.

4 Click **Add to Component 1** in the window toolbar.

5 In the **Home** toolbar, click **Add Physics** to close the **Add Physics** window.

EVENTS (EV)

Discrete States 1

1 Right-click **Component 1 (comp1)>Events (ev)** and choose **Discrete States**.

2 In the **Settings** window for **Discrete States**, locate the **Discrete States** section.

3 In the table, enter the following settings:

Name	Initial value (u0)	Description
V_max	1.8	Maximum voltage

Charge-discharge cycle

1 In the **Physics** toolbar, click **Global** and choose **Event Sequence**.

2 In the **Settings** window for **Event Sequence**, type `Charge-discharge cycle` in the **Label** text field.

3 Locate the **Sequence Control** section. Select the **Loop** check box.

Constant current

1 In the **Model Builder** window, expand the **Charge-discharge cycle** node, then click **Sequence Member 1**.

2 In the **Settings** window for **Sequence Member**, type `Constant current` in the **Label** text field.

3 Locate the **Sequence Member** section. In the **Discrete state name** text field, type `CC`.

4 In the **End condition expression (>0)** text field, type `comp1.right_el(phis)-V_max[V]`.

Charge-discharge cycle

In the **Model Builder** window, click **Charge-discharge cycle**.

Constant voltage

1 In the **Physics** toolbar, click **Attributes** and choose **Sequence Member**.

2 In the **Settings** window for **Sequence Member**, type `Constant voltage` in the **Label** text field.

3 Locate the **Sequence Member** section. In the **Discrete state name** text field, type `CV`.

4 From the **End condition** list, choose **Duration**.

5 In the **Duration** text field, type `t_cv`.

Charge-discharge cycle

In the **Model Builder** window, click **Charge-discharge cycle**.

Rest

1 In the **Physics** toolbar, click **Attributes** and choose **Sequence Member**.

Set the reinitialization value for V_max to V_max+0.2 to ramp up the maximum potential by 0.2[V] at the end of each cycle.

2 In the **Settings** window for **Sequence Member**, type `Rest` in the **Label** text field.

3 Locate the **Sequence Member** section. In the **Discrete state name** text field, type `REST`.

4 From the **End condition** list, choose **Duration**.

5 In the **Duration** text field, type `t_rest`.

6 Locate the **Reinitialization** section. In the table, enter the following settings:

Variable	Expression
V_max	V_max+0.2

TERTIARY CURRENT DISTRIBUTION, NERNST-PLANCK (TCD)

Set up the global equation for the applied current.

1 Click the **Show More Options** button in the **Model Builder** toolbar.

2 In the **Show More Options** dialog box, select **Physics>Equation-Based Contributions** in the tree.

3 In the tree, select the check box for the node **Physics>Equation-Based Contributions**.

4 Click **OK**.

Global Equations 1

1 In the **Model Builder** window, right-click **Tertiary Current Distribution, Nernst-Planck (tcd)** and choose **Global>Global Equations**.

2 In the **Settings** window for **Global Equations**, locate the **Global Equations** section.

3 In the table, enter the following settings:

Name	f(u,ut,utt,t) (I)	Initial value (u_0) (I)	Initial value (u_t0) (I/s)	Description
i_app_ch	(CC==1)*(i_app_ch-i_app)/i_app+(CV==1)*(right_el(phis)-V_min)/V_min+(REST==1)*(i_app_ch)/i_app	i_app	0	

4 Locate the **Units** section. Click **Define Dependent Variable Unit**.

5 In the **Dependent variable quantity** table, enter the following settings:

Dependent variable quantity	Unit
Custom unit	A

Electrode Current Density 1, Global Equations 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Tertiary Current Distribution, Nernst-Planck (tcd)**, Ctrl-click to select **Electrode Current Density 1** and **Global Equations 1**.

2 Right-click and choose **Group**.

Constant Current Charge/Constant Voltage Discharge

In the **Settings** window for **Group**, type `Constant Current Charge/Constant Voltage Discharge` in the **Label** text field.

MESH 1

Define the user-controlled mesh.

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

2 In the **Settings** window for **Mesh**, locate the **Sequence Type** section.

3 From the list, choose **User-controlled mesh**.

Size 1

1 In the **Model Builder** window, right-click **Edge 1** and choose **Size**.

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

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

4 From the **Selection** list, choose **All boundaries**.

5 Locate the **Element Size** section. From the **Predefined** list, choose **Extremely fine**.

6 Click **Build All**.

STUDY 1: CC CHARGE CV DISCHARGE

Set up the time-dependent study for the electrochemical cell for the load cycle defined as events.

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

2 In the **Settings** window for **Study**, type `Study 1: CC Charge CV Discharge` 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, under **Study 1: CC Charge CV Discharge** click **Step 1: Time Dependent**.

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

3 From the **Time unit** list, choose **min**.

4 In the **Output times** text field, type `0 40`.

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 In the **Model Builder** window, expand the **Study 1: CC Charge CV Discharge> Solver Configurations>Solution 1 (sol1)>Dependent Variables 1** node, then click **State variable i_app_ch (comp1.ODE1)**.

4 In the **Settings** window for **State**, locate the **Scaling** section.

5 From the **Method** list, choose **Manual**.

6 In the **Scale** text field, type `i_app`.

7 In the **Model Builder** window, under **Study 1: CC Charge CV Discharge> Solver Configurations>Solution 1 (sol1)** click **Time-Dependent Solver 1**.

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

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

10 Click to expand the **Time Stepping** section. From the **Steps taken by solver** list, choose **Strict**.

11 Select the **Initial step** check box.

12 In the **Event tolerance** text field, type `0.001`.

13 Click to expand the **Results While Solving** section. Right-click **Study 1: CC Charge CV Discharge>Solver Configurations>Solution 1 (sol1)>Time-Dependent Solver 1** and choose **Stop Condition**.

Add the stop condition for the time-dependent solver to stop at 2.45 [V].

14 In the **Model Builder** window, expand the **Study 1: CC Charge CV Discharge> Solver Configurations>Solution 1 (sol1)>Time-Dependent Solver 1** node, then click **Stop Condition 1**.

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

16 Click + **Add**.

17 In the table, enter the following settings:

Stop expression	Stop if	Active	Description
`comp1.V_max>2.45`	True (>=1)	√	`Stop expression 1`

18 Locate the **Output at Stop** section. From the **Add solution** list, choose **Steps before and after stop**.

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

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

RESULTS

Voltage and Current Profile for CC Charge - CV Discharge

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

2 In the **Settings** window for **1D Plot Group**, type `Voltage and Current Profile for CC Charge - CV Discharge` in the **Label** text field.

Current

1 Right-click **Voltage and Current Profile for CC Charge - CV Discharge** and choose **Global**.

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

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

Expression	Unit	Description
`comp1.i_app_ch`	A	`Cell Current`

4 Locate the **x-Axis Data** section. From the **Unit** list, choose **s**.

5 In the **Voltage and Current Profile for CC Charge - CV Discharge** toolbar, click **Plot**.

Potential

1 In the **Model Builder** window, right-click **Voltage and Current Profile for CC Charge - CV Discharge** and choose **Point Graph**.

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

3 Select Boundary 4 only.

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

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

6 Locate the **x-Axis Data** section. From the **Unit** list, choose **s**.

7 Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dash-dot**.

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

9 Find the **Include** subsection. Clear the **Point** check box.

10 Clear the **Expression** check box.

11 Select the **Description** check box.

Voltage and Current Profile for CC Charge - CV Discharge

1 In the **Model Builder** window, click **Voltage and Current Profile for CC Charge - CV Discharge**.

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 **Current**.

5 In the **Model Builder** window, click **Voltage and Current Profile for CC Charge - CV Discharge**.

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

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

8 In the **Voltage and Current Profile for CC Charge - CV Discharge** toolbar, click **Plot**.

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

Voltage and Current Profile for CC Charge - CV Discharge (Overlapped)

1 Right-click **Voltage and Current Profile for CC Charge - CV Discharge** and choose **Duplicate**.

2 In the **Settings** window for **1D Plot Group**, type `Voltage and Current Profile for CC Charge - CV Discharge (Overlapped)` in the **Label** text field.

Current

1 In the **Model Builder** window, expand the **Voltage and Current Profile for CC Charge - CV Discharge (Overlapped)** node, then click **Current**.

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

3 From the **Parameter** list, choose **Expression**.

4 In the **Expression** text field, type `t-t_REST_start-t_rest`.

Filter 1

1 Right-click **Current** and choose **Filter**.

2 In the **Settings** window for **Filter**, locate the **Point Selection** section.

3 In the **Logical expression for inclusion** text field, type `(REST!=1)&&(V_max>1.8)`.

4 Locate the **Line Segment Selection** section. Clear the **Decreasing x** check box.

Color Expression 1

1 Right-click **Current** and choose **Color Expression**.

2 In the **Settings** window for **Color Expression**, locate the **Expression** section.

3 In the **Expression** text field, type `V_max`.

4 Locate the **Coloring and Style** section. Clear the **Color legend** check box.

Potential

1 In the **Model Builder** window, under **Results>Voltage and Current Profile for CC Charge - CV Discharge (Overlapped)** click **Potential**.

2 In the **Settings** window for **Point Graph**, locate the **x-Axis Data** section.

3 From the **Parameter** list, choose **Expression**.

4 In the **Expression** text field, type `t-t_REST_start-t_rest`.

Filter 1

1 Right-click **Potential** and choose **Filter**.

2 In the **Settings** window for **Filter**, locate the **Point Selection** section.

3 In the **Logical expression for inclusion** text field, type `(REST!=1)&&(V_max>1.8)`.

4 Locate the **Line Segment Selection** section. Clear the **Decreasing x** check box.

Color Expression 1

1 Right-click **Potential** and choose **Color Expression**.

2 In the **Settings** window for **Color Expression**, locate the **Expression** section.

3 In the **Expression** text field, type `V_max`.

4 Locate the **Coloring and Style** section. Clear the **Color legend** check box.

Voltage and Current Profile for CC Charge - CV Discharge (Overlapped)

1 In the **Model Builder** window, expand the **Results>**
Voltage and Current Profile for CC Charge - CV Discharge (Overlapped) node, then click **Voltage and Current Profile for CC Charge - CV Discharge (Overlapped)**.

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

3 Select the **Manual axis limits** check box.

4 In the **x minimum** text field, type `0`.

5 In the **x maximum** text field, type `40`.

6 In the **y minimum** text field, type `0`.

7 In the **y maximum** text field, type `2.6`.

8 In the **Secondary y minimum** text field, type `-2000`.

9 In the **Secondary y maximum** text field, type `300`.

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

11 In the **Voltage and Current Profile for CC Charge - CV Discharge (Overlapped)** toolbar, click **Plot**.

TERTIARY CURRENT DISTRIBUTION, NERNST-PLANCK (TCD)

Define the constant power charge condition for the electrochemical capacitor.

Electrode Power 1

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

2 Select Boundary 4 only.

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

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

5 In the p_{average} text field, type `-P_app/A_cell`.

6 In the $\phi_{\text{s,bnd,init}}$ text field, type `V_rest`.

Initial Values - Constant Power

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

2 Select Domain 3 only.

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

4 In the *c*2 text field, type `c_bulk`.

5 In the *phis* text field, type `V_rest`.

6 In the **Label** text field, type `Initial Values - Constant Power`.

Electrode Power 1, Initial Values - Constant Power

1 In the **Model Builder** window, under **Component 1 (comp1)>Tertiary Current Distribution, Nernst-Planck (tcd)**, Ctrl-click to select **Electrode Power 1** and **Initial Values - Constant Power**.

2 Right-click and choose **Group**.

Constant Power Charge

1 In the **Settings** window for **Group**, type `Constant Power Charge` in the **Label** text field.

Set up the study for the constant power charge.

ADD STUDY

1 In the **Home** toolbar, click **Add Study** to open the **Add Study** window.

2 Go to the **Add Study** window.

3 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies> Time Dependent**.

4 Click **Add Study** in the window toolbar.

5 In the **Home** toolbar, click **Add Study** to close the **Add Study** window.

STUDY 2

Step 1: Time Dependent

1 In the **Settings** window for **Time Dependent**, locate the **Physics and Variables Selection** section.

2 Select the **Modify model configuration for study step** check box.

3 In the tree, select **Component 1 (comp1)>Tertiary Current Distribution, Nernst-Planck (tcd)>Constant Current Charge/Constant Voltage Discharge**.

4 Right-click and choose **Disable**.

5 In the tree, select **Component 1 (comp1)>Events (ev)**.

6 Click **Disable in Model**.

7 Locate the **Study Settings** section. In the **Output times** text field, type `0 2`.

Solution 2 (sol2)

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

Step 1: Time Dependent

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

2 In the **Settings** window for **Time Dependent**, click to expand the **Study Extensions** section.

3 Clear all domains.

4 Select the **Auxiliary sweep** check box.

5 Click **Add**.

6 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
P_app (Applied Power)	`0.5[kW] 0.85[kW]`	`W`

7 Click **Add**.

8 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
V_rest (Rest potential for applied power)	`-2.1[V] -2.5[V]`	`V`

9 In the **Model Builder** window, click **Study 2**.

10 In the **Settings** window for **Study**, type `Study 2: Constant Power Charge` in the **Label** text field.

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

Solution 2 (sol2)

1 In the **Model Builder** window, expand the **Study 2: Constant Power Charge> Solver Configurations>Solution 2 (sol2)** node, then click **Time-Dependent Solver 1**.

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

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

Step 1: Time Dependent

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

RESULTS

Double Layer Current

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

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

3 Locate the **Title** section. From the **Title type** list, choose **Label**.

Line Graph 1

1 Right-click **Double Layer Current** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, locate the **Selection** section.

3 Click to select the **Activate Selection** toggle button.

4 Select Domains 1 and 3 only.

5 Locate the **Data** section. From the **Dataset** list, choose **Study 2: Constant Power Charge/ Solution 2 (sol2)**.

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

7 Locate the **y-Axis Data** section. In the **Expression** text field, type `tcd.ivdl`.

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

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

10 In the **Double Layer Current** toolbar, click **Plot**.

11 Select the **Description** check box. In the associated text field, type `Dimensionless length`.

12 In the **Double Layer Current** toolbar, click **Plot**.

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

Double Layer Current

1 In the **Model Builder** window, click **Double Layer Current**.

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

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

4 In the **Double Layer Current** toolbar, click **Plot**.

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

Charge Density for Charging Power

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

Plot the charge density using the concentration from depositing-dissolving species node.

2 In the **Settings** window for **1D Plot Group**, type `Charge Density for Charging Power` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 2: Constant Power Charge/ Solution 2 (sol2)**.

4 From the **Time selection** list, choose **Last**.

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

Line Graph 1

1 Right-click **Charge Density for Charging Power** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, locate the **Selection** section.

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

4 Click to expand the **y-Axis Data** section. In the **Expression** text field, type `-tcd.c_pce1_c1_q*F_const`.

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

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

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

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

Charge Density for Charging Power

1 In the **Model Builder** window, click **Charge Density for Charging Power**.

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 `Dimensionless length (1)`.

4 Click to expand the **Legend** section. From the **Position** list, choose **Upper left**.

5 In the **Charge Density for Charging Power** toolbar, click **Plot**.

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

Voltage and Current Profiles for Constant Power 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 `Voltage and Current Profiles for Constant Power Charge` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 2: Constant Power Charge/Solution 2 (sol2)**.

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

Current

1 Right-click **Voltage and Current Profiles for Constant Power Charge** and choose **Point Graph**.

2 In the **Settings** window for **Point Graph**, type `Current` in the **Label** text field.

3 Select Boundary 4 only.

4 Locate the **y-Axis Data** section. In the **Expression** text field, type `right_el(tcd.nIs)*A_cell`.

5 Locate the **Legends** section. Select the **Show legends** check box.

6 Locate the **Coloring and Style** section. From the **Color** list, choose **Cycle (reset)**.

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

8 In the **Legend** text field, type `Current (P = eval(P_app) kW)`.

9 In the **Voltage and Current Profiles for Constant Power Charge** toolbar, click **Plot**.

Potential

1 In the **Model Builder** window, right-click **Voltage and Current Profiles for Constant Power Charge** and choose **Global**.

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

3 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> tcd.phis0_epow1 - Electric potential on boundary - V**.

4 Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dash-dot**.

5 From the **Color** list, choose **Cycle (reset)**.

6 Click to expand the **Legends** section. From the **Legends** list, choose **Evaluated**.

7 In the **Legend** text field, type `Potential (P = eval(P_app) kW)`.

8 In the **Voltage and Current Profiles for Constant Power Charge** toolbar, click **Plot**.

Voltage and Current Profiles for Constant Power Charge

1 In the **Model Builder** window, click **Voltage and Current Profiles for Constant Power Charge**.

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

3 Select the **y-axis label** check box. In the associated text field, type `Current (A)`.

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

5 Select the **Secondary y-axis label** check box. In the associated text field, type `Electric Potential (V)`.

6 In the table, select the **Plot on secondary y-axis** check box for **Potential**.

7 In the **Voltage and Current Profiles for Constant Power Charge** toolbar, click **Plot**.

8 Locate the **Axis** section. Clear the **Manual axis limits** check box.

9 In the **Model Builder** window, click **Voltage and Current Profiles for Constant Power Charge**.

10 Select the **Manual axis limits** check box.

11 In the **y minimum** text field, type `200.79068524910107`.

12 In the **y maximum** text field, type `340.58128603840646`.

13 In the **Voltage and Current Profiles for Constant Power Charge** toolbar, click **Plot**.

14 In the **Secondary y maximum** text field, type `-0.45314923375307226`.

15 In the **Secondary y minimum** text field, type `-3`.

16 In the **Voltage and Current Profiles for Constant Power Charge** toolbar, click **Plot**.

17 Locate the **Legend** section. From the **Position** list, choose **Center**.

18 In the **Voltage and Current Profiles for Constant Power Charge** toolbar, click **Plot**.