



Model created in COMSOL Multiphysics 6.4

Capacitive Deionization of Saline Water

Introduction

Desalination is the removal of salt (NaCl) from, for example, brine or seawater to obtain water suitable for human use. Efficient production of potable water from seawater is useful in parts of the world where freshwater access is limited. One method for desalination is capacitive deionization, where the sodium and chloride ions in seawater are driven into porous electrodes by an external applied electrical potential. This model shows how to implement the improved modified Donnan model for capacitive deionization in a “flow-between” capacitive deionization cell.

Model Definition

GEOMETRY

The geometry of the system is shown in [Figure 1](#).

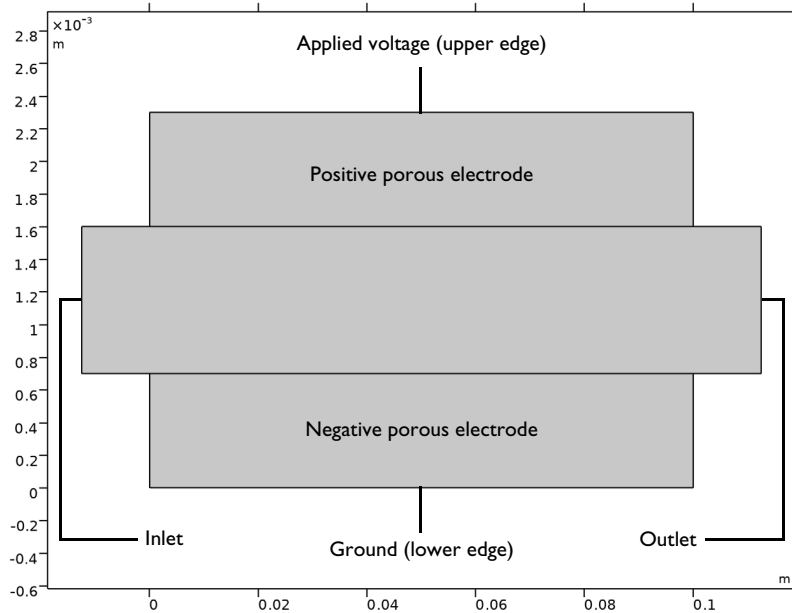


Figure 1: Geometry of the capacitive deionization system. For clarity, the y-axis has been scaled by a factor of 30.

The inlet is located at the left-most vertical boundary and the outlet at the corresponding right-hand side vertical boundary. The main flow channel, from the inlet to the outlet, is bracketed by the two horizontal porous electrodes. The upper, positive, porous electrode

is connected to the external circuit along its upper boundary, and the lower, negative, porous electrode is connected to the external circuit along its lower boundary.

FLUID FLOW

The flow through the open main channel, and through the porous electrodes, is described using a **Brinkman Equations** interface. The flow field is solved for independently of the deionization process, and the flow field is then used in a **Tertiary Current Distribution, Nernst–Planck** interface.

ELECTROCHEMISTRY

The Tertiary Current Distribution, Nernst–Planck interface solves for the electrode and electrolyte electric potentials, as well as for the concentrations of the Na^+ and Cl^- ions. Electroneutrality is assumed in the electrolyte. A Porous Electrode node is used to describe the transport of species and charge in the porous electrode domains. A more detailed description of the governing equations of this interface can be found in the documentation for the [Wire Electrode](#) tutorial.

Improved Modified Donnan Model

In this model, the ions are driven, by the applied potential, and by a nonelectrostatic attractive force, into micropores inside the porous electrodes. This process reduces the salt concentration in the water exiting the cell (deionization). The deionization process is modeled using the “improved modified Donnan” model of Bazant and coworkers ([Ref. 1](#)). The improved modified Donnan model extends the Donnan equilibrium model by introducing a concentration- and micropore size-dependent attractive potential between the micropore walls and the ions inside the micropores of the porous electrode. The micropores are assumed to be homogeneously distributed inside the porous electrodes. It is assumed that all capacitive effects are localized to these micropores.

To derive the relationship between the ionic concentrations inside the micropores and the macropores of the porous electrodes, electrochemical equilibrium between the micro- and macropores is assumed:

$$\bar{\mu}_{i, \text{mi}} = \bar{\mu}_{i, \text{l}} \quad (1)$$

In [Equation 1](#), the subscript “ i ” refers to a species index, “mi” refers to “micropore”, and the subscript “l” refers to the liquid electrolyte. In [Equation 1](#), $\bar{\mu}_i$ is the electrochemical potential of species i (J/mol). Applying the definition of the electrochemical potential allows for rewriting [Equation 1](#) in terms of concentrations (c_i , mol/m³), electrical potentials (ϕ , V), and the previously mentioned nonelectrostatic attractive potential ($\mu_{\text{att},i}$, J/mol). For the macropore electrolyte,

$$\bar{\mu}_{i,l} = \mu_{i,l} + z_i F \phi_l \quad (2)$$

and for the micropore electrolyte,

$$\bar{\mu}_{i,mi} = \mu_{i,mi} + z_i F \phi_{mi} - \mu_{att,i} \quad (3)$$

In Equation 2 and Equation 3, μ_i is the chemical potential of species i , z_i is the charge of species i , and F is Faraday's constant (C/mol). The attractive potential is assumed to be the same for all ions, and to be given by

$$\mu_{att,i} = \mu_{att} = \frac{E}{\sum c_{i,mi}} \quad (4)$$

Here, the attractive volumetric energy density E (J/m³) is given by

$$E = z^2 k_B T \lambda_B \lambda_p^{-4} \quad (5)$$

where z is the ionic charge, k_B is Boltzmann's constant (J/K), T is the temperature (K), λ_B is the Bjerrum length in the micropore (m) and λ_p is the micropore size (m).

By assuming unit activity (a_i , dimensionless), the chemical potential can be rewritten in terms of concentration as

$$\mu_i = \mu_i^\circ + RT \log a_i = \mu_i^\circ + RT \log c_i \quad (6)$$

In Equation 6, R is the molar gas constant (J/K/mol). Substituting these expressions into Equation 1, and rearranging, gives the Donnan condition

$$c_{i,mi} = c_{i,l} e^{\left(\frac{z_i F}{RT}(\phi_l - \phi_{mi}) + \mu_{att}\right)} \quad (7)$$

An additional expression is needed to determine the micropore electrolyte potential ϕ_{mi} . That expression is the macropore-micropore current balance

$$\frac{d(C(\phi_s - \phi_{mi}))}{dt} = \frac{d\left(-\epsilon_{mi} F \sum z_i c_{i,mi}\right)}{dt} \quad (8)$$

In Equation 8, C is the volumetric capacitance (F/m³)

$$C = C_{ref} + \alpha \left(\sum z_i c_{i,mi}\right)^2 \quad (9)$$

where C_{ref} (F/m^3) and α (the pore charge to surface capacitance ratio, $\text{F}\cdot\text{m}^3/\text{mol}^2$) are experimentally determined parameters, and ε_{mi} is the volume fraction of micropores (dimensionless).

Finally, the volume-averaged source/sink term R_i ($\text{mol}/(\text{m}^3\cdot\text{s})$), defining the flux of ions from macropore to micropore, is written as

$$R_i = -\varepsilon_{\text{mi}} \frac{dc_{i,\text{mi}}}{dt} \quad (10)$$

Current Efficiency

The charge efficiency, H (dimensionless), of the process is determined, for the charging part of the process (between 1980 s and 5220 s), using the following expression

$$H = \frac{-\Gamma F}{\Sigma} \quad (11)$$

where Γ is the cumulative amount of salt stored in the micropores (mol) and Σ is the cumulative electrical charge passed through the external circuit (C). Specifically,

$$\frac{d\Gamma}{dt} = Q(c_{i,\text{in}} - c_{i,\text{out}}) \quad (12)$$

where Q is the inlet volumetric flow rate (m^3/s), and

$$\frac{d\Sigma}{dt} = \oint_{\partial\Omega_{\text{upper}}} (n \cdot \mathbf{i}_s) dS \quad (13)$$

In [Equation 13](#), the surface integral is evaluated only for the top boundary of the upper porous electrode, and \mathbf{i}_s is the electrode current density (A/m^2).

Results and Discussion

The flow through the cell is shown in [Figure 2](#). The flow velocity in the porous electrodes is much lower than that in the main channel.

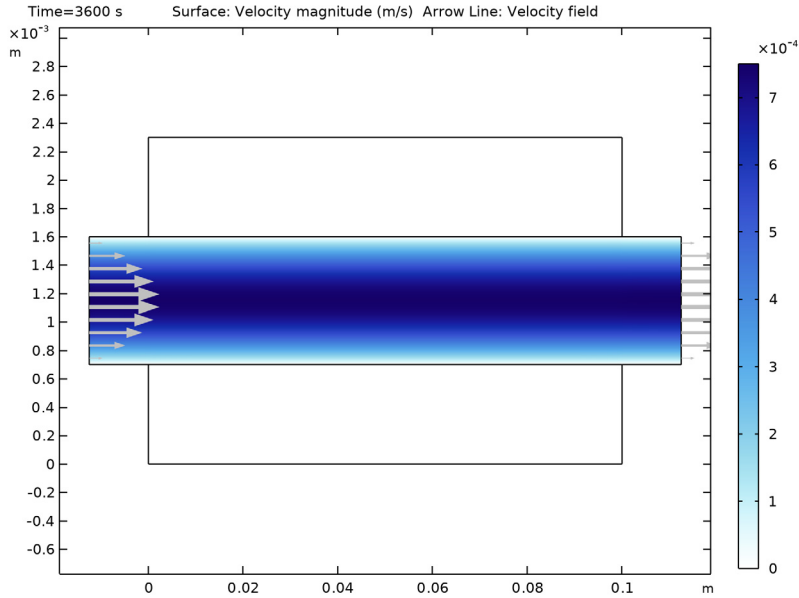


Figure 2: The flow through the cell.

The simulation starts with both terminals being connected without any external load (0 V applied potential). Next, at 1800 s, a positive voltage of 0.4 V is applied on the top (positive) porous electrode. The lower electrode is assumed to be connected to ground. Finally, the external applied voltage is again turned off. [Figure 3](#) shows the flow averaged outlet concentration during the capacitive deionization process. The outlet concentration is highly time dependent.

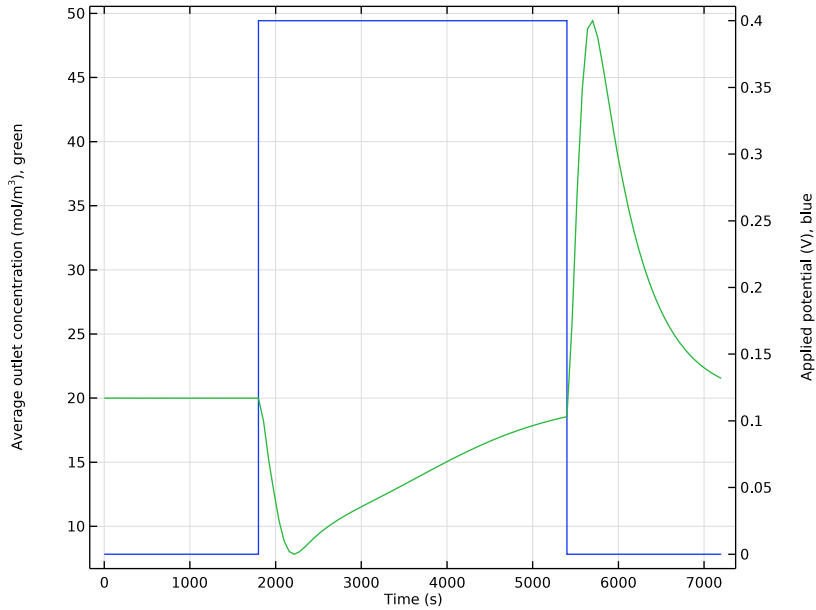


Figure 3: The mixing-cup average outlet salt concentration during the simulation.

Figure 3 shows that during the charging process, as the micropore concentrations increase toward the value given by the Donnan condition, the outlet concentration gradually approaches the inlet value. The variation in the micropore concentration of Cl^- during the simulation is shown in Figure 4. During the charging part of the simulation, the amount of Cl^- increases in the upper (positive) electrode, while the lower (negative) electrode is emptied. The concentrations gradually approach a saturation value. When the voltage is again set to 0 V, the micropore concentrations approach a value similar to the starting concentrations.

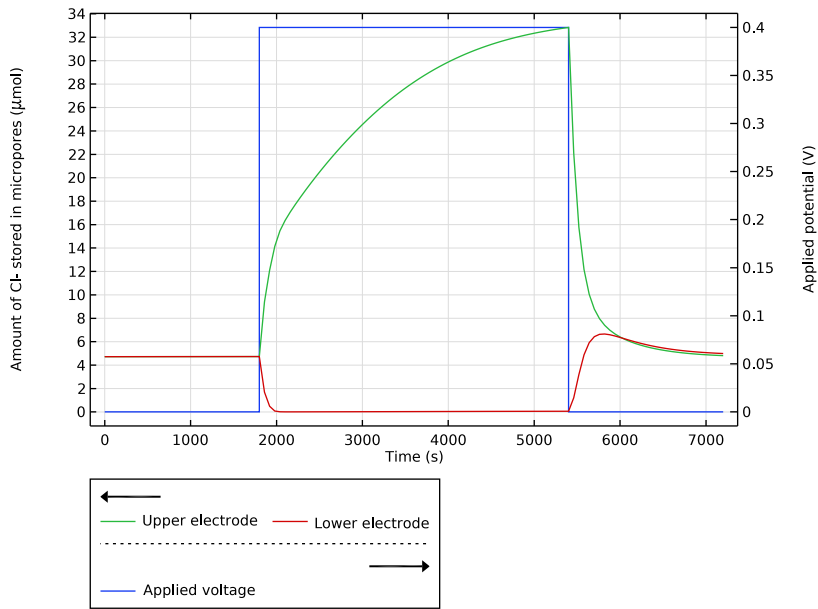


Figure 4: The micropore amount of Cl^- ions during the process.

Figure 5 shows the desalination ratio throughout the macropores and main channel after 3600 s. At the outlet, the salt concentration has been reduced to about half of the inlet concentration.

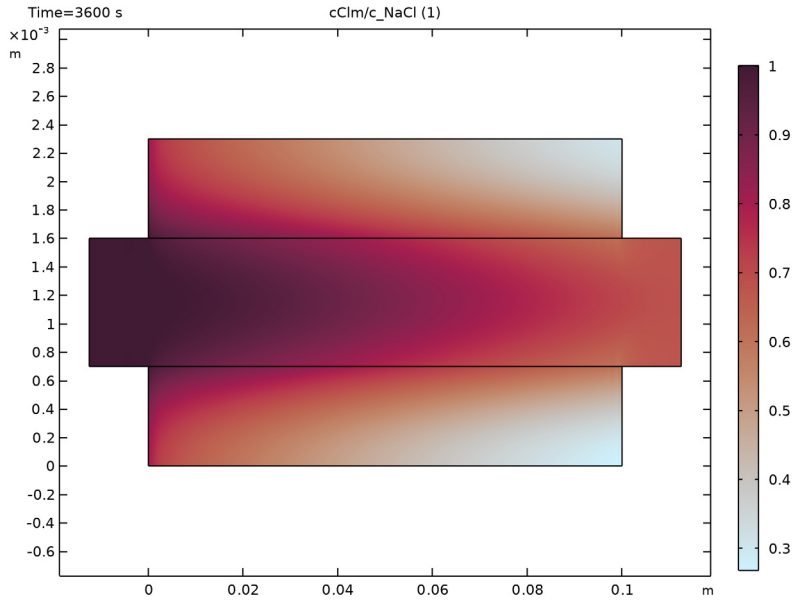


Figure 5: The desalination ratio in the electrolyte, in macropores and the main channel, after 3600 s. The desalination ratio varies significantly between different parts of the porous electrodes.

The maximum and minimum values of the local attractive potential, μ_{att} , and capacitance are shown in Figure 6 and Figure 7, respectively, both for the upper electrode. The two quantities vary significantly during the simulation.

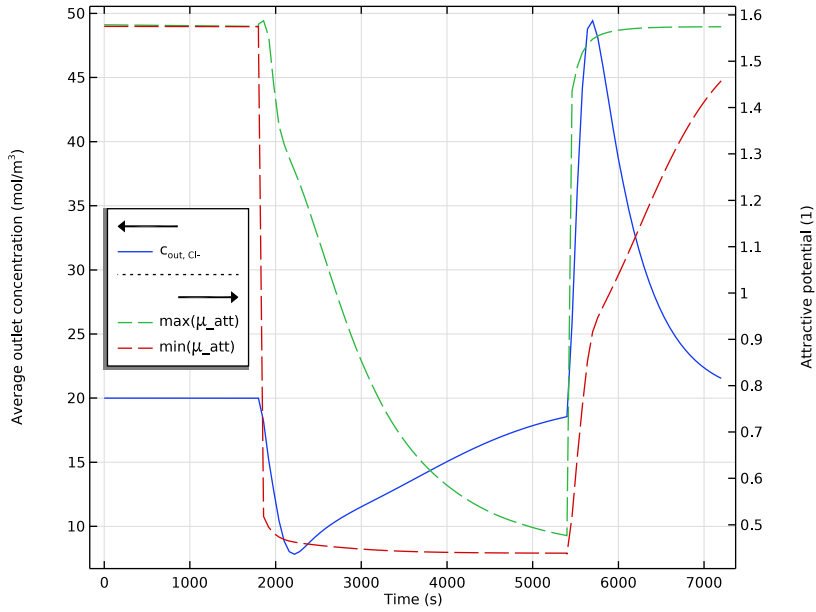


Figure 6: The maximum and minimum values for the local attractive potential in the upper electrode.

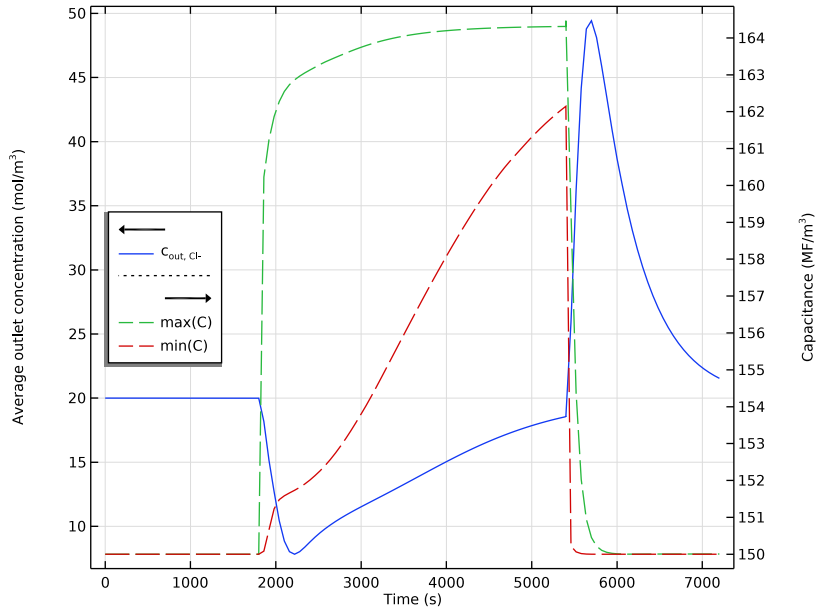


Figure 7: The maximum and minimum values for the local capacitance in the upper electrode.

Finally, the charge efficiency during the charging part of the process is shown in [Figure 8](#). The efficiency increases toward a value of 70%.

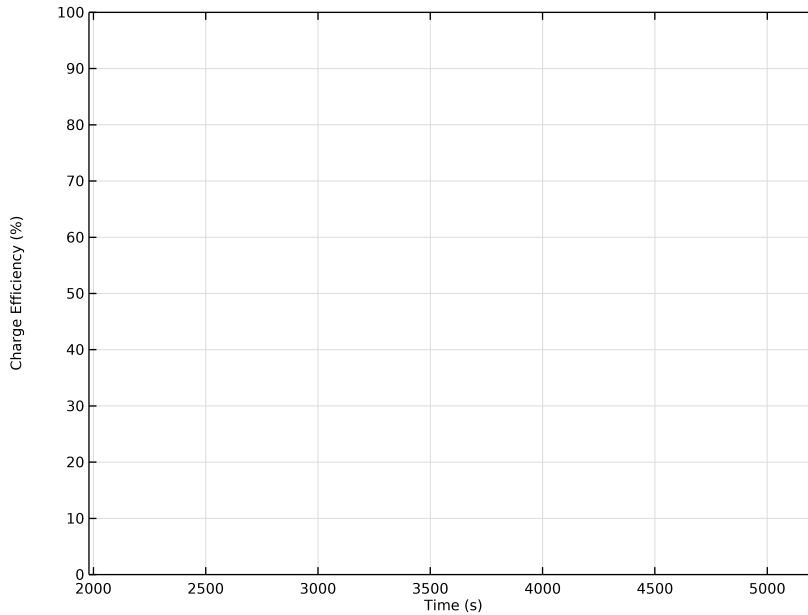


Figure 8: Charge efficiency during desalination.

Notes About the COMSOL Implementation

As the deionization process is assumed to be completely non-Faradaic, the Porous Electrode Reaction subnode under the Tertiary Current Distribution, Nernst–Planck, Porous Electrode 1 node is disabled.

The coupling between micro- and macropores is carried out through a Reactions node, where the flux according to [Equation 10](#) is entered.

[Equation 5](#) is solved for in the **Domain ODEs and DAEs: Attractive Potential** interface, and [Equation 8](#) is solved for in the **Domain ODEs and DAEs: Micropore Electrolyte Potential** interface. The charge efficiency ([Equation 11](#)) is computed as a postprocessing operation, in the **Evaluation Group: Charge Efficiency** evaluation group.

References


1. P.M. Biesheuvel, S. Porada, M. Levi, and M.Z. Bazant, “Attractive forces in microporous carbon electrodes for capacitive deionization,” *J. Solid State Electrochem.*, vol. 18, pp. 1365–1376, 2014.
2. A. Hemmatifar, M. Stadermann, and J.G. Santiago, “Two-Dimensional Porous Electrode Model for Capacitive Deionization,” *J. Phys. Chem. C*, vol. 119, pp. 24681–24694, 2015.

Application Library path: Electrochemistry_Module/
Electrochemical_Engineering/capacitive_deionization


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  **2D**.
- 2 In the **Select Physics** tree, select **Electrochemistry > Tertiary Current Distribution, Nernst–Planck > Tertiary, Electroneutrality (tcd)**.
- 3 Click **Add**.
- 4 In the **Concentrations (mol/m³)** table, enter the following settings:

cNap
cClm
- 5 In the **Select Physics** tree, select **Fluid Flow > Porous Media and Subsurface Flow > Brinkman Equations (br)**.
- 6 Click **Add**.
- 7 In the **Select Physics** tree, select **Mathematics > ODE and DAE Interfaces > Domain ODEs and DAEs (dode)**.
- 8 Click **Add**.

9 In the **Field name (I)** text field, type `phil_micro`.

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

<code>phil_micro</code>

11 Click  **Define Dependent Variable Unit**.

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

Dependent variable quantity	Unit
Custom unit	V

13 In the **Source term quantity** table, enter the following settings:

Source term quantity	Unit
Custom unit	A/m ³

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

15 Click **Add**.

16 In the **Source term quantity** table, enter the following settings:

Source term quantity	Unit
Custom unit	1

17 In the **Field name (I)** text field, type `mu`.

18 In the **Dependent variables (I)** table, enter the following settings:

<code>mu</code>

19 Click  **Study**.

20 In the **Select Study** tree, select **General Studies > Stationary**.


21 Click  **Done**.

GLOBAL DEFINITIONS

Geometry



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

2 In the **Settings** window for **Parameters**, type `Geometry` 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 `capacitive_deionization_geometry.txt`.



Electrolyte

- 1 In the **Home** toolbar, click  **Parameters** and choose **Add > Parameters**.
- 2 In the **Settings** window for **Parameters**, type `Electrolyte` 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 `capacitive_deionization_electrolyte.txt`.



Porous Electrode

- 1 In the **Home** toolbar, click  **Parameters** and choose **Add > Parameters**.
- 2 In the **Settings** window for **Parameters**, type `Porous Electrode` 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 `capacitive_deionization_porous_electrode.txt`.



Porous Electrode, Attractive Potential

- 1 In the **Home** toolbar, click  **Parameters** and choose **Add > Parameters**.
- 2 In the **Settings** window for **Parameters**, type `Porous Electrode, Attractive Potential` 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 `capacitive_deionization_porous_electrode_attractive_potential.txt`.

Flow



- 1 In the **Home** toolbar, click  **Parameters** and choose **Add > Parameters**.
- 2 In the **Settings** window for **Parameters**, type `Flow` 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 `capacitive_deionization_flow.txt`.

Process

- 1 In the **Home** toolbar, click  **Parameters** and choose **Add > Parameters**.
- 2 In the **Settings** window for **Parameters**, type `Process` 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 `capacitive_deionization_process.txt`.



Mesh

- 1 In the **Home** toolbar, click  **Parameters** and choose **Add > Parameters**.
- 2 In the **Settings** window for **Parameters**, type Mesh 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 `capacitive_deionization_mesh.txt`.


Next, define the variables, a function, nonlocal couplings and view settings needed for the model. Some of the variables and nonlocal couplings will show warnings, since we have not yet defined the geometry.

DEFINITIONS

Donnan Condition and Current Balance

- 1 In the **Home** toolbar, click  **Variables** and choose **Local Variables**.
- 2 In the **Settings** window for **Variables**, type Donnan Condition and Current Balance in the **Label** text field.
- 3 Locate the **Variables** section. Click  **Load from File**.
- 4 Browse to the model's Application Libraries folder and double-click the file `capacitive_deionization_donnan_condition_current_balance.txt`.

Outlet Concentration

- 1 In the **Home** toolbar, click  **Variables** and choose **Local Variables**.
- 2 In the **Settings** window for **Variables**, type Outlet Concentration in the **Label** text field.
- 3 Locate the **Variables** section. In the table, enter the following settings:

Name	Expression	Unit	Description
c_out_Cl _m	$\text{intop_outlet}(\text{tcd.ntf lux_cClm} \cdot d_z) / \text{intop_outlet}(u \cdot d_z)$		Outlet concentration, Cl ⁻
c_out_Na _p	$\text{intop_outlet}(\text{tcd.ntf lux_cNap} \cdot d_z) / \text{intop_outlet}(u \cdot d_z)$		Outlet concentration, Na ⁺

Porous Electrode, Attractive Potential

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

2 In the **Settings** window for **Variables**, type Porous Electrode, Attractive Potential in the **Label** text field.

3 Locate the **Variables** section. In the table, enter the following settings:

Name	Expression	Unit	Description
csum	cNap_micro+cClm_micro	mol/m ³	Sum of micropore concentrations
mu_att	E/csum/ root.k_B_const/T/ root.N_A_const		Nonelectrostatic adsorption potential

Porous Electrode, Stern Layer Properties

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

2 In the **Settings** window for **Variables**, type Porous Electrode, Stern Layer Properties in the **Label** text field.

3 Locate the **Variables** section. In the table, enter the following settings:

Name	Expression	Unit	Description
C	C_ref+alpha*charge_sum^2	s ⁴ ·A ² /(kg·m ⁵)	Stern layer capacitance

Storage

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

2 In the **Settings** window for **Variables**, type Storage in the **Label** text field.

3 Locate the **Variables** section. In the table, enter the following settings:

Name	Expression	Unit	Description
n_Clm_upper	intop_upper_electrode(cClm_micro*d_z)		Amount of Cl ⁻ , upper electrode
n_Clm_lower	intop_lower_electrode(cClm_micro*d_z)		Amount of Cl ⁻ , lower electrode

Define two integration operators, one for the upper and one for the lower electrode. They will be used to compute the total amount of stored Cl⁻ in each electrode.

Integration 1 (intop1)

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


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

Integration 2 (intop_upper_electrode2)


- 1 Right-click **Integration 1 (intop_upper_electrode)** and choose **Duplicate**.
- 2 In the **Settings** window for **Integration**, type `intop_lower_electrode` in the **Operator name** text field.

Define a maximum and a minimum operator. They will be used to plot the maximum and minimum value of the local attractive potential and local capacitance in the upper electrode.

Maximum 1 (maxop1)


- 1 In the **Definitions** toolbar, click  **Nonlocal Couplings** and choose **Maximum**.
- 2 In the **Settings** window for **Maximum**, type `maxop_upper` in the **Operator name** text field.

Minimum 1 (minop1)

- 1 In the **Definitions** toolbar, click  **Nonlocal Couplings** and choose **Minimum**.
- 2 In the **Settings** window for **Minimum**, type `minop_upper` in the **Operator name** text field.

Define an integration operator for the outlet. It will be used to compute the mixing-cup average outlet concentration of salt.

Integration, outlet boundary


- 1 In the **Definitions** toolbar, click  **Nonlocal Couplings** and choose **Integration**.
- 2 In the **Settings** window for **Integration**, type `Integration, outlet boundary` in the **Label** text field.
- 3 In the **Operator name** text field, type `intop_outlet`.

Axis

- 1 In the **Model Builder** window, expand the **Component 1 (comp1) > Definitions > View 1** node, then click **Axis**.
- 2 In the **Settings** window for **Axis**, locate the **Axis** section.
- 3 From the **View scale** list, choose **Manual**.
- 4 In the **y scale** text field, type 30.


GEOMETRY 1

Rectangle 1 (r1)


- 1 In the **Geometry** toolbar, click  **Rectangle**.
- 2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
- 3 In the **Width** text field, type `L_electrode`.

4 In the **Height** text field, type h_{porous} .


Rectangle 2 (r2)

- 1 In the **Geometry** toolbar, click  **Rectangle**.
- 2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
- 3 In the **Width** text field, type $L_{\text{electrode}}$.
- 4 In the **Height** text field, type h_{gap} .
- 5 Locate the **Position** section. In the **y** text field, type h_{porous} .


Rectangle 3 (r3)

- 1 In the **Geometry** toolbar, click  **Rectangle**.
- 2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
- 3 In the **Width** text field, type $L_{\text{electrode}}$.
- 4 In the **Height** text field, type h_{porous} .
- 5 Locate the **Position** section. In the **y** text field, type $h_{\text{porous}}+h_{\text{gap}}$.



Rectangle 4 (r4)



- 1 In the **Geometry** toolbar, click  **Rectangle**.
- 2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
- 3 In the **Width** text field, type L_{pipe} .
- 4 In the **Height** text field, type h_{gap} .
- 5 Locate the **Position** section. In the **x** text field, type $-L_{\text{pipe}}$.
- 6 In the **y** text field, type h_{porous} .

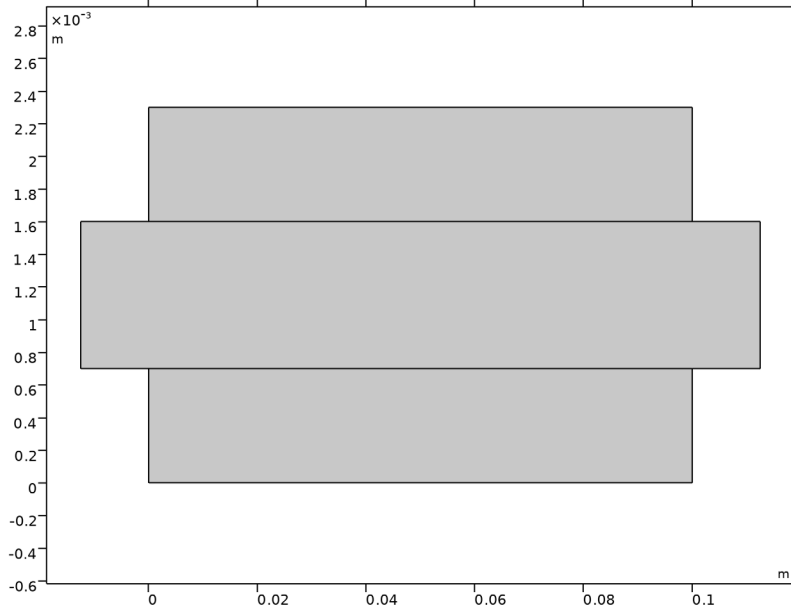
Rectangle 5 (r5)

- 1 In the **Geometry** toolbar, click  **Rectangle**.
- 2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
- 3 In the **Width** text field, type L_{pipe} .
- 4 In the **Height** text field, type h_{gap} .
- 5 Locate the **Position** section. In the **x** text field, type $L_{\text{electrode}}$.
- 6 In the **y** text field, type h_{porous} .

Ignore Edges 1 (ige1)

- 1 In the **Geometry** toolbar, click  **Virtual Operations** and choose **Ignore Edges**.
- 2 In the **Settings** window for **Ignore Edges**, locate the **Input** section.
- 3 Click the  **Paste Selection** button for **Edges to ignore**.

- 4 In the **Paste Selection** dialog, type 6, 12 in the **Selection** text field.
- 5 Click **OK**.
- 6 In the **Geometry** toolbar, click  **Build All**.
- 7 Click the  **Zoom Extents** button in the **Graphics** toolbar.



Now that the geometry has been defined, set the correct selections on the nonlocal coupling operators.

DEFINITIONS

Integration 1 (intop_upper_electrode)

- 1 In the **Model Builder** window, under **Component 1 (comp1) > Definitions** click **Integration 1 (intop_upper_electrode)**.
- 2 Select Domain 3 only.

Integration 2 (intop_lower_electrode)

- 1 In the **Model Builder** window, click **Integration 2 (intop_lower_electrode)**.
- 2 Select Domain 2 only.

Maximum 1 (maxop_upper)

- 1 In the **Model Builder** window, click **Maximum 1 (maxop_upper)**.

2 Select Domain 3 only.

Minimum 1 (minop_upper)

1 In the **Model Builder** window, click **Minimum 1 (minop_upper)**.

2 Select Domain 3 only.

Integration, outlet boundary (intop_outlet)

1 In the **Model Builder** window, click **Integration, outlet boundary (intop_outlet)**.

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

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

4 Select Boundary 14 only.

All the warnings should now have disappeared.

Next, add material properties for the saline solution.

ADD MATERIAL

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

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

3 In the tree, select **Built-in > Water, liquid**.

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

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

MATERIALS

Water, liquid (mat1)

A few properties are not defined in the water material properties, but we will define those later in the corresponding physics interfaces instead.

Now, define the settings in the physics interfaces

TERTIARY CURRENT DISTRIBUTION, NERNST-PLANCK (TCD)

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**, locate the **Out-of-Plane Thickness** section.

3 In the d_z text field, type d_z .

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_{cNap} text field, type z_Nap .
- 4 In the z_{cClm} text field, type z_Clm .


Electrolyte 1

- 1 In the **Model Builder** window, click **Electrolyte 1**.
- 2 In the **Settings** window for **Electrolyte**, locate the **Convection** section.
- 3 From the **u** list, choose **Velocity field (br)**.
- 4 Locate the **Diffusion** section. In the D_{cNap} text field, type DNa .
- 5 In the D_{cClm} text field, type DCl .

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 $cClm$ text field, type c_NaCl .

Porous Electrode 1


- 1 In the **Physics** toolbar, click  **Domains** and choose **Porous Electrode**.
- 2 Select Domains 2 and 3 only.
- 3 In the **Settings** window for **Porous Electrode**, locate the **Convection** section.
- 4 From the **u** list, choose **Velocity field (br)**.
- 5 Locate the **Diffusion** section. In the D_{cNap} text field, type DNa .
- 6 In the D_{cClm} text field, type DCl .
- 7 Locate the **Electrode Current Conduction** section. From the σ_s list, choose **User defined**.
Define an arbitrary, but high, electrical conductivity for the porous electrode. In the associated text field, type 100.
- 8 Locate the **Porous Matrix Properties** section. In the ϵ_s text field, type eps_s .
- 9 In the ϵ_l text field, type $1 - eps_s$.

Porous Electrode Reaction 1

Disable the Porous Electrode Reaction subnode. Faradaic reactions will not be taken into account in the present model.

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

Inflow 1

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Inflow**.
- 2 Select Boundary 1 only.
- 3 In the **Settings** window for **Inflow**, locate the **Concentration** section.
- 4 In the $c_{0,cClm}$ text field, type `root.c_NaCl`.


Outflow 1

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Outflow**.
- 2 Select Boundary 14 only.


Electric Ground 1

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Electric Ground**.
- 2 Select Boundary 5 only.

Load Cycle 1

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Load Cycle**.
- 2 Select Boundary 9 only.
- 3 In the **Settings** window for **Load Cycle**, locate the **Load Type** section.
- 4 From the list, choose **Potentiostatic**.
- 5 Locate the **Continuation Conditions** section. Select the **Use elapsed time only** checkbox.


Voltage 1

- 1 In the **Physics** toolbar, click  **Attributes** and choose **Voltage**.
- 2 In the **Settings** window for **Voltage**, locate the **Continuation Conditions** section.
- 3 Select the **Elapsed time** checkbox.
- 4 In the t_{max} text field, type `30[min]`.

Load Cycle 1

In the **Model Builder** window, click **Load Cycle 1**.

Voltage 2

- 1 In the **Physics** toolbar, click  **Attributes** and choose **Voltage**.
- 2 In the **Settings** window for **Voltage**, locate the **Voltage** section.
- 3 In the E_{set} text field, type `V_max`.
- 4 Locate the **Continuation Conditions** section. Select the **Elapsed time** checkbox.

Load Cycle 1

In the **Model Builder** window, click **Load Cycle 1**.

Voltage 3

In the **Physics** toolbar, click  **Attributes** and choose **Voltage**.

Reactions 1

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

To couple the micropore and macropore concentrations in the porous electrodes, add a Reactions node as follows:

- 2 Select Domains 2 and 3 only.
- 3 In the **Settings** window for **Reactions**, locate the **Reaction Rates** section.
- 4 In the R_{cNap} text field, type `R_Nap_macro`.
- 5 In the R_{cClm} text field, type `R_Cl_m_macro`.
- 6 Click to expand the **Reacting Volume** section. From the list, choose **Total volume**.

BRINKMAN EQUATIONS (BR)

Porous Matrix 1

- 1 In the **Model Builder** window, under **Component 1 (comp1) > Brinkman Equations (br) > Porous Medium 1** click **Porous Matrix 1**.
- 2 In the **Settings** window for **Porous Matrix**, locate the **Matrix Properties** section.
- 3 From the ϵ_p list, choose **User defined**. In the associated text field, type `eps_s`.
- 4 From the κ list, choose **User defined**. In the associated text field, type `kappa_s`.

Initial Values 1


- 1 In the **Model Builder** window, under **Component 1 (comp1) > Brinkman Equations (br)** click **Initial Values 1**.
- 2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.
- 3 Specify the **u** vector as

u_{in}	x
----------	-----

Fluid Properties 1


- 1 In the **Physics** toolbar, click  **Domains** and choose **Fluid Properties**.
- 2 Select Domain 1 only.

Inlet 1

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Inlet**.
- 2 Select Boundary 1 only.
- 3 In the **Settings** window for **Inlet**, locate the **Boundary Condition** section.

- 4 From the list, choose **Fully developed flow**.
- 5 Locate the **Fully Developed Flow** section. In the U_{av} text field, type u_{in} .

Outlet 1

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Outlet**.
- 2 Select Boundary 14 only.
Enable Normal flow to simulate that the pipe continues on the other side of the system boundary.
- 3 In the **Settings** window for **Outlet**, locate the **Pressure Conditions** section.
- 4 Select the **Normal flow** checkbox.

Define the settings of the Global ODEs and DAEs interface used to compute the micropore electrolyte potential as follows:

DOMAIN ODES AND DAES: MICROPORE ELECTROLYTE POTENTIAL

- 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: Micropore Electrolyte Potential in the **Label** text field.
- 3 Select Domains 2 and 3 only.
- 4 Click to expand the **Dependent Variables** section.

Distributed ODE 1

- 1 In the **Model Builder** window, under **Component 1 (comp1)** > **Domain ODEs and DAEs: Micropore Electrolyte Potential (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 $iv_d1_helmholtz-iv_d1_diffuse$.
- 4 Locate the **Damping or Mass Coefficient** section. In the d_a text field, type 0.

Define the settings of the Domain ODEs and DAEs interface used to compute the attractive potential.

DOMAIN ODES AND DAES: ATTRACTIVE POTENTIAL

- 1 In the **Model Builder** window, under **Component 1 (comp1)** click **Domain ODEs and DAEs 2 (dode2)**.
- 2 In the **Settings** window for **Domain ODEs and DAEs**, type Domain ODEs and DAEs: Attractive Potential in the **Label** text field.
- 3 Select Domains 2 and 3 only.

- 1 In the **Model Builder** window, under **Component 1 (comp1)** > **Domain ODEs and DAEs: Attractive Potential (dode2)** click **Distributed ODE 1**.
- 2 In the **Settings** window for **Distributed ODE**, locate the **Source Term** section.
- 3 In the f text field, type $\mu_{att} - \mu$.
- 4 Locate the **Damping or Mass Coefficient** section. In the d_a text field, type 0.

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 μ text field, type μ_0 .

As the geometry has only 90 degree angles, set up a mapped mesh.

MESH 1

- 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 In the **Model Builder** window, under **Component 1 (comp1)** > **Mesh 1** click **Size**.
- 2 In the **Settings** window for **Size**, locate the **Element Size** section.
- 3 From the **Calibrate for** list, choose **General physics**.
- 4 From the **Predefined** list, choose **Normal**.


Boundary Layers 1, Corner Refinement 1, Free Triangular 1, Size 1

- 1 In the **Model Builder** window, under **Component 1 (comp1)** > **Mesh 1**, Ctrl-click to select **Size 1**, **Corner Refinement 1**, **Free Triangular 1**, and **Boundary Layers 1**.
- 2 Right-click and choose **Delete**.

Mapped 1


In the **Mesh** toolbar, click  **Mapped**.

Distribution 1


- 1 In the **Mesh** toolbar, click  **Distribution**.
- 2 Select Boundaries 7 and 12 only.
- 3 In the **Settings** window for **Distribution**, locate the **Distribution** section.
- 4 From the **Distribution type** list, choose **Predefined**.
- 5 In the **Number of elements** text field, type $elem_porous_count$.

6 In the **Element ratio** text field, type 2.


Distribution 2

- 1 In the **Mesh** toolbar, click  **Distribution**.
- 2 Select Boundaries 4 and 10 only.
- 3 In the **Settings** window for **Distribution**, locate the **Distribution** section.
- 4 From the **Distribution type** list, choose **Predefined**.
- 5 In the **Number of elements** text field, type `elem_porous_count`.
- 6 In the **Element ratio** text field, type 2.
- 7 Select the **Reverse direction** checkbox.

Distribution 3

- 1 In the **Mesh** toolbar, click  **Distribution**.
- 2 Select Boundaries 5 and 9 only.
- 3 In the **Settings** window for **Distribution**, locate the **Distribution** section.
- 4 From the **Distribution type** list, choose **Predefined**.
- 5 In the **Number of elements** text field, type `elem_length_count`.

Distribution 4


- 1 In the **Mesh** toolbar, click  **Distribution**.
- 2 Select Boundaries 1 and 14 only.
- 3 In the **Settings** window for **Distribution**, locate the **Distribution** section.
- 4 From the **Distribution type** list, choose **Predefined**.
- 5 In the **Number of elements** text field, type `elem_pipe_count`.
- 6 In the **Element ratio** text field, type 2.
- 7 Select the **Symmetric distribution** checkbox.

STUDY 1

Step 1: Stationary



- 1 In the **Model Builder** window, under **Study 1** click **Step 1: Stationary**.
- 2 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.
- 3 In the **Solve for** column of the table, under **Component 1 (comp1)**, clear the checkboxes for **Tertiary Current Distribution, Nernst–Planck (tcd)**, **Domain ODEs and DAEs: Micropore Electrolyte Potential (dode)**, and **Domain ODEs and DAEs: Attractive Potential (dode2)**.

Step 2: Time Dependent

- 1 In the **Study** toolbar, click  **Time Dependent**.
- 2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.
- 3 In the **Output times** text field, type 0 range (30[**min**], 1[**min**], 2[**h**]).
- 4 Locate the **Physics and Variables Selection** section. In the **Solve for** column of the table, under **Component 1 (comp1)**, clear the checkbox for **Brinkman Equations (br)**.

To reduce the computation time, change to the Constant (Newton) nonlinear method, on the Fully Coupled node.


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 > Solver Configurations > Solution 1 (sol1) > Time-Dependent Solver 1** node, then click **Fully Coupled 1**.
- 4 In the **Settings** window for **Fully Coupled**, click to expand the **Method and Termination** section.
- 5 From the **Nonlinear method** list, choose **Constant (Newton)**.
The model setup is now complete. Compute the study.
- 6 In the **Study** toolbar, click  **Compute**.

Next, add a single-select configuration, for 3600 s, and improve the default plots.

RESULTS

Single-Select Solution 1

- 1 In the **Results** toolbar, click  **Configurations** and choose **Single-Select Solution**.
- 2 In the **Settings** window for **Single-Select Solution**, locate the **Solution** section.
- 3 From the **Time (s)** list, choose **Interpolation**.
- 4 In the **Time** text field, type 3600.


Electrolyte Potential (tcd)

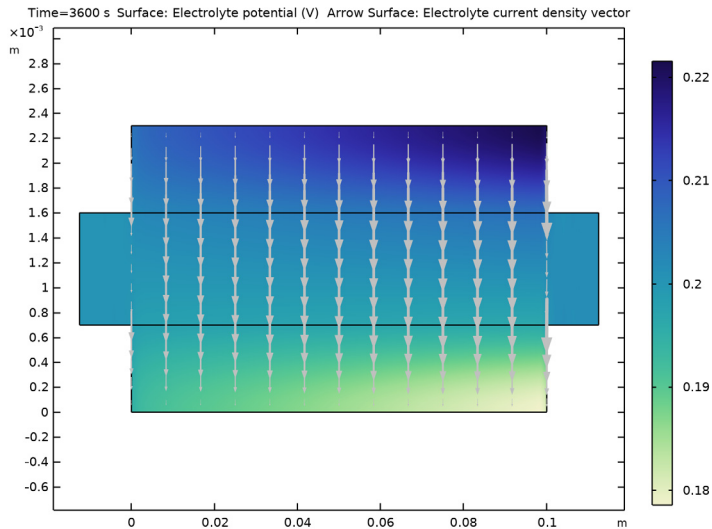
- 1 In the **Model Builder** window, under **Results** click **Electrolyte Potential (tcd)**.
- 2 In the **Settings** window for **2D Plot Group**, locate the **Data** section.
- 3 From the **Solution parameters** list, choose **From configuration**.

Surface 1

- 1 In the **Model Builder** window, expand the **Electrolyte Potential (tcd)** node, then click **Surface 1**.
- 2 In the **Settings** window for **Surface**, locate the **Coloring and Style** section.
- 3 From the **Color table** list, choose **Cyanthus**.

Arrow Surface 1

- 1 In the **Model Builder** window, click **Arrow Surface 1**.
- 2 In the **Settings** window for **Arrow Surface**, locate the **Coloring and Style** section.
- 3 Select the **Scale factor** checkbox. In the associated text field, type 0.005.
- 4 In the **Electrolyte Potential (tcd)** toolbar, click  **Plot**.



Electrolyte Current Density (tcd)

In the **Model Builder** window, under **Results** right-click **Electrolyte Current Density (tcd)** and choose **Delete**.


Electrode Potential with Respect to Ground (tcd)

- 1 In the **Model Builder** window, expand the **Results >** **Electrode Potential with Respect to Ground (tcd)** node, then click **Electrode Potential with Respect to Ground (tcd)**.
- 2 In the **Settings** window for **2D Plot Group**, locate the **Data** section.
- 3 From the **Solution parameters** list, choose **From configuration**.

Surface 1

- 1 In the **Model Builder** window, click **Surface 1**.
- 2 In the **Settings** window for **Surface**, locate the **Coloring and Style** section.
- 3 From the **Color table** list, choose **Cynanthus**.

Arrow Surface 1

- 1 In the **Model Builder** window, click **Arrow Surface 1**.
- 2 In the **Settings** window for **Arrow Surface**, locate the **Coloring and Style** section.
- 3 Select the **Scale factor** checkbox. In the associated text field, type 0.005.
- 4 In the **Electrode Potential with Respect to Ground (tcd)** toolbar, click  **Plot**.

Electrode Current Density (tcd)

In the **Model Builder** window, under **Results** right-click **Electrode Current Density (tcd)** and choose **Delete**.


Concentration, Nap (tcd)


- 1 In the **Settings** window for **2D Plot Group**, locate the **Data** section.
- 2 From the **Solution parameters** list, choose **From configuration**.

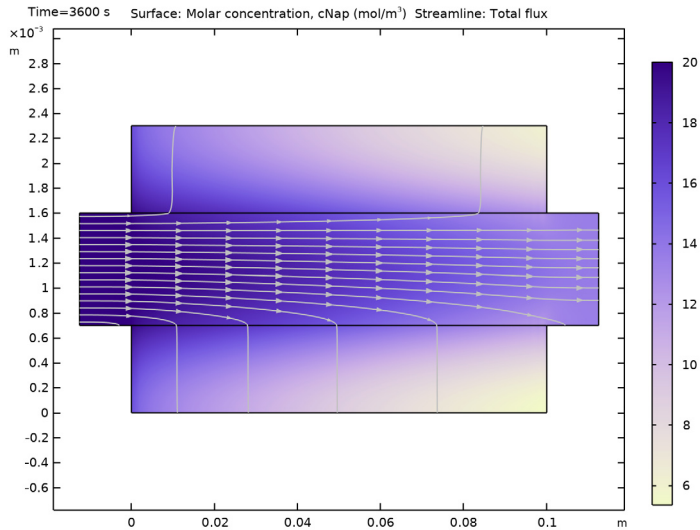
Surface 1

- 1 In the **Model Builder** window, expand the **Concentration, Nap (tcd)** node, then click **Surface 1**.
- 2 In the **Settings** window for **Surface**, locate the **Coloring and Style** section.
- 3 From the **Color table** list, choose **Baptisia**.

Streamline 1

- 1 In the **Model Builder** window, click **Streamline 1**.
- 2 In the **Settings** window for **Streamline**, locate the **Streamline Positioning** section.
- 3 From the **Positioning** list, choose **On selected boundaries**.
- 4 In the **Number** text field, type 16.
- 5 Locate the **Selection** section. Click to select the  **Activate Selection** toggle button.
- 6 Select Boundary 1 only.
- 7 Locate the **Coloring and Style** section. Find the **Point style** subsection.
- 8 Select the **Scale factor** checkbox. In the associated text field, type 0.5.

9 In the **Concentration, Nap (tcd)** toolbar, click  **Plot**.



Concentration, Clm (tcd)


- 1 In the **Model Builder** window, under **Results** click **Concentration, Clm (tcd)**.
- 2 In the **Settings** window for **2D Plot Group**, locate the **Data** section.
- 3 From the **Solution parameters** list, choose **From configuration**.

Surface 1

- 1 In the **Model Builder** window, expand the **Concentration, Clm (tcd)** node, then click **Surface 1**.
- 2 In the **Settings** window for **Surface**, locate the **Coloring and Style** section.
- 3 From the **Color table** list, choose **Baptisia**.

Streamline 1

- 1 In the **Model Builder** window, click **Streamline 1**.
- 2 In the **Settings** window for **Streamline**, locate the **Streamline Positioning** section.
- 3 From the **Positioning** list, choose **On selected boundaries**.
- 4 In the **Number** text field, type 16.
- 5 Locate the **Selection** section. Click to select the **Activate Selection** toggle button.
- 6 Select Boundary 1 only.
- 7 Locate the **Coloring and Style** section. Find the **Point style** subsection.

- 8 Select the **Scale factor** checkbox. In the associated text field, type 0.5.
- 9 In the **Concentration, Clm (tcd)** toolbar, click  **Plot**.


Velocity (br)

- 1 In the **Model Builder** window, under **Results** click **Velocity (br)**.
- 2 In the **Settings** window for **2D Plot Group**, locate the **Data** section.
- 3 From the **Solution parameters** list, choose **From configuration**.

Surface

- 1 In the **Model Builder** window, expand the **Velocity (br)** node, then click **Surface**.
- 2 In the **Settings** window for **Surface**, locate the **Coloring and Style** section.
- 3 From the **Color table** list, choose **Kyanite**.



Velocity (br)


In the **Velocity (br)** toolbar, click  **Arrow Line**.

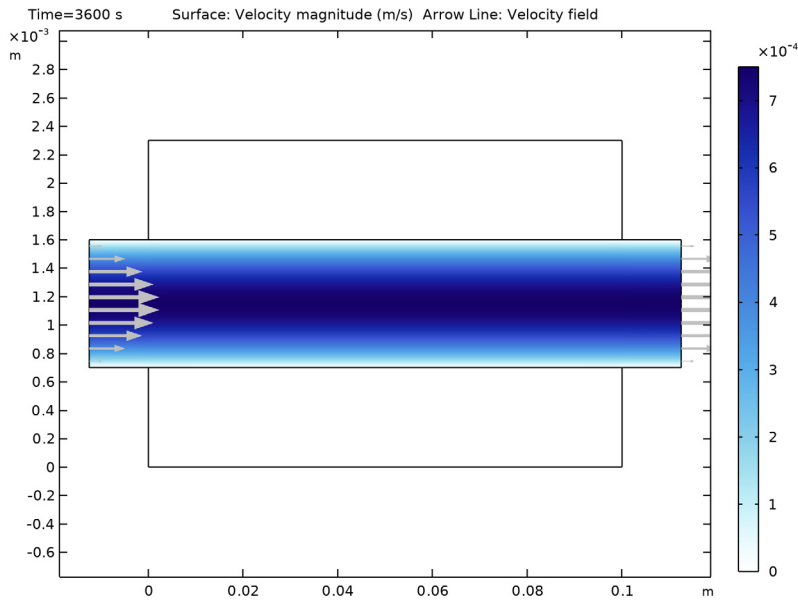
Arrow Line 1

- 1 In the **Settings** window for **Arrow Line**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1) > Brinkman Equations > Velocity and pressure > u,v - Velocity field**.
- 2 Locate the **Arrow Positioning** section. From the **Placement** list, choose **Uniform anisotropic**.
- 3 In the **Number of arrows** text field, type 20.
- 4 Locate the **Coloring and Style** section.
- 5 Select the **Scale factor** checkbox. In the associated text field, type 20.
- 6 From the **Color** list, choose **Gray**.

Selection 1

- 1 In the **Velocity (br)** toolbar, click  **Selection**.
- 2 In the **Settings** window for **Selection**, locate the **Selection** section.
- 3 Click  **Paste Selection**.
- 4 In the **Paste Selection** dialog, type 1 14 in the **Selection** text field.
- 5 Click **OK**.

6 In the **Velocity (br)** toolbar, click  **Plot**.



Pressure (br)

- 1 In the **Model Builder** window, under **Results** click **Pressure (br)**.
- 2 In the **Settings** window for **2D Plot Group**, locate the **Data** section.
- 3 From the **Solution parameters** list, choose **From configuration**.

Domain ODEs and DAEs: Micropore Electrolyte Potential

- 1 In the **Model Builder** window, click **Domain ODEs and DAEs: Micropore Electrolyte Potential**.
- 2 In the **Settings** window for **2D Plot Group**, locate the **Data** section.
- 3 From the **Solution parameters** list, choose **From configuration**.

Surface I

- 1 In the **Model Builder** window, expand the **Domain ODEs and DAEs: Micropore Electrolyte Potential** node, then click **Surface I**.
- 2 In the **Settings** window for **Surface**, locate the **Coloring and Style** section.
- 3 From the **Color table** list, choose **Cyanthus**.


Domain ODEs and DAEs: Attractive Potential

- 1 In the **Model Builder** window, under **Results** click **Domain ODEs and DAEs: Attractive Potential**.
- 2 In the **Settings** window for **2D Plot Group**, locate the **Data** section.
- 3 From the **Solution parameters** list, choose **From configuration**.


Surface 1


- 1 In the **Model Builder** window, expand the **Domain ODEs and DAEs: Attractive Potential** node, then click **Surface 1**.
- 2 In the **Settings** window for **Surface**, locate the **Coloring and Style** section.
- 3 From the **Color table** list, choose **Arctium**.

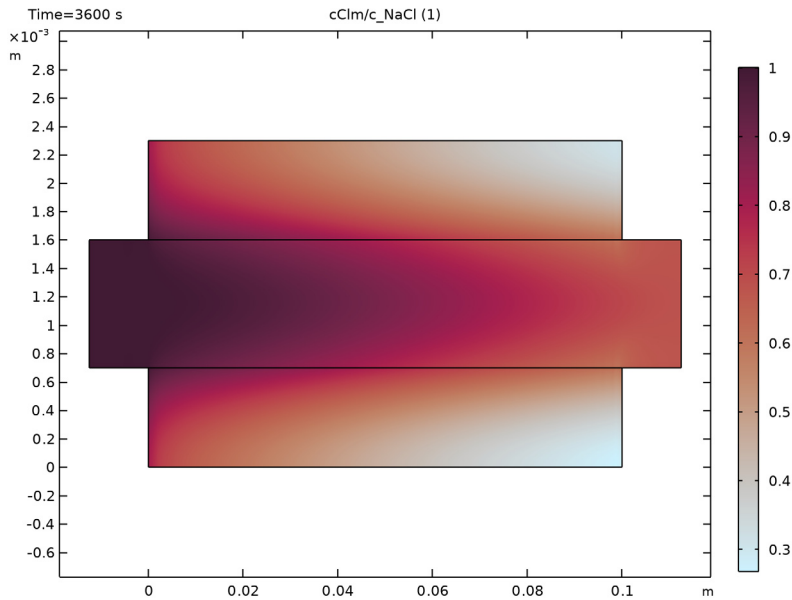
Salinity Ratio

- 1 In the **Results** toolbar, click  **2D Plot Group**.
- 2 In the **Settings** window for **2D Plot Group**, type Salinity Ratio in the **Label** text field.
- 3 Locate the **Data** section. From the **Solution parameters** list, choose **From configuration**.


Surface 1

- 1 In the **Salinity Ratio** toolbar, click  **Surface**.
- 2 In the **Settings** window for **Surface**, locate the **Expression** section.
- 3 In the **Expression** text field, type $c_{Cl}m/c_{NaCl}$.
- 4 Locate the **Coloring and Style** section. From the **Color table** list, choose **MetasepiaBlue**.


5 In the **Salinity Ratio** toolbar, click  **Plot**.



Mixing-Cup Average Outlet Salt Concentration

- 1 In the **Home** toolbar, click  **Add Plot Group** and choose **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, type Mixing-Cup Average Outlet Salt Concentration in the **Label** text field.
- 3 Click to expand the **Title** section. From the **Title type** list, choose **None**.
- 4 Locate the **Plot Settings** section.
- 5 Select the **y-axis label** checkbox. In the associated text field, type Average outlet concentration (mol/m^3), green.
- 6 Select the **Two y-axes** checkbox.
- 7 Select the **Secondary y-axis label** checkbox. In the associated text field, type Applied potential (V), blue.
- 8 Locate the **Legend** section. Clear the **Show legends** checkbox.

Applied Potential


- 1 In the **Mixing-Cup Average Outlet Salt Concentration** toolbar, click  **Global**.
- 2 In the **Settings** window for **Global**, type Applied Potential in the **Label** text field.
- 3 Locate the **y-Axis** section. Select the **Plot on secondary y-axis** checkbox.

- Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component I (comp1) > Tertiary Current Distribution, Nernst–Planck > Load Cycle I > tcd.lcl.E_app - Applied voltage - V**.

Mixing-Cup Average Outlet Salt Concentration

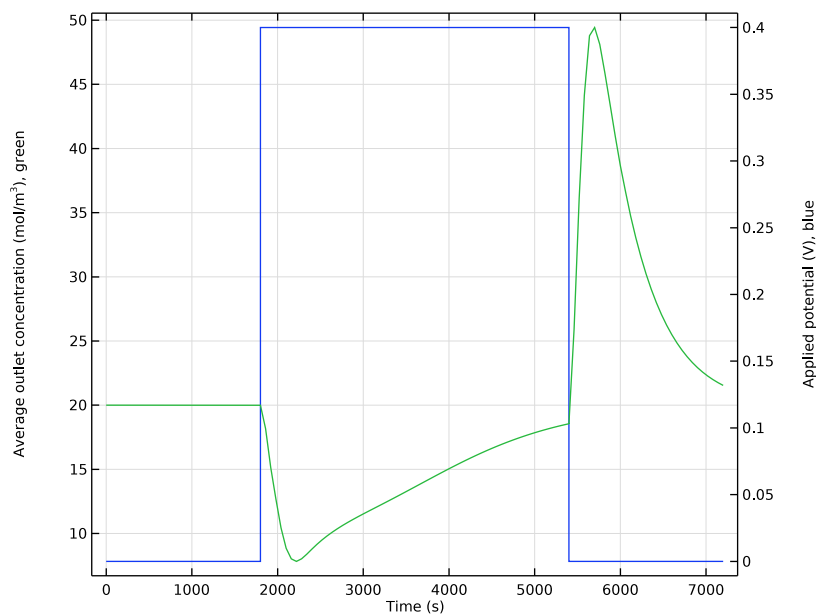
In the **Mixing-Cup Average Outlet Salt Concentration** toolbar, click  **Global**.

Outlet Concentration

- In the **Settings** window for **Global**, type Outlet Concentration in the **Label** text field.
- Locate the **y-Axis Data** section. Click  **Clear Table**.
- In the table, enter the following settings:

Expression	Unit	Description
c_out_C1m	mol/m ³	Outlet concentration, Cl-

- In the **Mixing-Cup Average Outlet Salt Concentration** toolbar, click  **Plot**.



Mixing-Cup Average Outlet Salt Concentration and mu

- In the **Model Builder** window, right-click **Mixing-Cup Average Outlet Salt Concentration** and choose **Duplicate**.
- In the **Model Builder** window, click **Mixing-Cup Average Outlet Salt Concentration 1**.

- 3 In the **Settings** window for **ID Plot Group**, type **Mixing-Cup Average Outlet Salt Concentration** and **mu** in the **Label** text field.
- 4 Locate the **Plot Settings** section. In the **y-axis label** text field, type **Average outlet concentration (mol/m³)**.
- 5 In the **Secondary y-axis label** text field, type **Attractive potential (1)**.
- 6 Locate the **Legend** section. Select the **Show legends** checkbox.
- 7 From the **Position** list, choose **Middle left**.

Applied Potential

In the **Model Builder** window, right-click **Applied Potential** and choose **Delete**.

Outlet Concentration

- 1 In the **Settings** window for **Global**, click to expand the **Legends** section.
- 2 From the **Legends** list, choose **Manual**.
- 3 In the table, enter the following settings:

Legends
c _{out} , Cl-

Mixing-Cup Average Outlet Salt Concentration and mu

In the **Mixing-Cup Average Outlet Salt Concentration and mu** toolbar, click  **Global**.

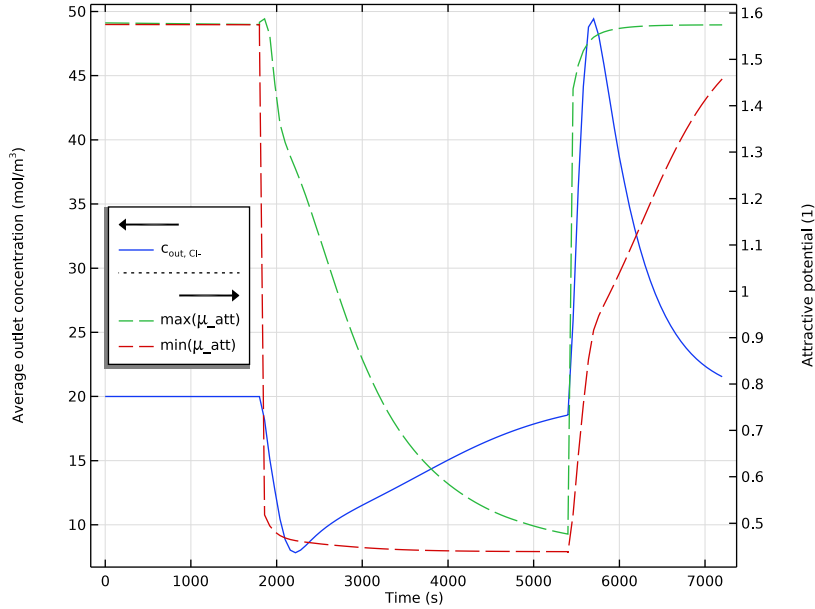
Max and min \mu_{att}, upper electrode

- 1 In the **Settings** window for **Global**, type **Max and min \mu_{att}, upper electrode** in the **Label** text field.
- 2 Locate the **y-Axis** section. Select the **Plot on secondary y-axis** checkbox.
- 3 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
maxop_upper(mu_att)	1	max(\mu _{att})
minop_upper(mu_att)	1	min(\mu _{att})

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

5 In the **Mixing-Cup Average Outlet Salt Concentration and mu** toolbar, click  **Plot**.



Mixing-Cup Average Outlet Salt Concentration and C

- 1 In the **Model Builder** window, right-click **Mixing-Cup Average Outlet Salt Concentration and mu** and choose **Duplicate**.
- 2 In the **Settings** window for **ID Plot Group**, type Mixing-Cup Average Outlet Salt Concentration and C in the **Label** text field.
- 3 Locate the **Plot Settings** section. In the **Secondary y-axis label** text field, type Capacitance (MF/m³).

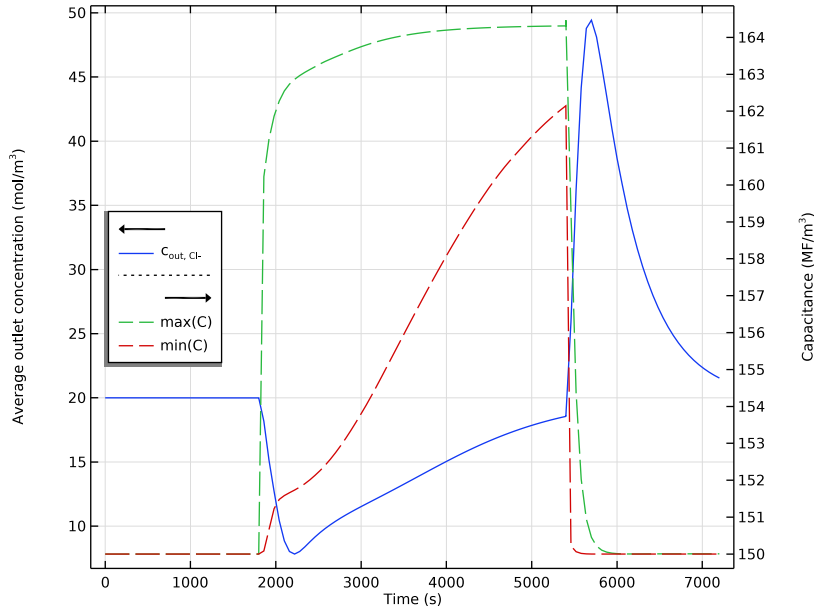
Max and min C, upper electrode

- 1 In the **Model Builder** window, expand the **Mixing-Cup Average Outlet Salt Concentration and C** node, then click **Max and min μ_{att} , upper electrode**.
- 2 In the **Settings** window for **Global**, type Max and min C, upper electrode in the **Label** text field.

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


Expression	Unit	Description
maxop_upper(C)	MF/m ³	max(C)
minop_upper(C)	MF/m ³	min(C)

4 In the **Mixing-Cup Average Outlet Salt Concentration and C** toolbar, click  **Plot**.




Define an evaluation group, used to compute the amount of salt stored and the charge passed through the external circuit. Together, these two quantities define the charge efficiency of the cell.

Evaluation Group: Charge Efficiency

- 1 In the **Results** toolbar, click  **Evaluation Group**.
- 2 In the **Settings** window for **Evaluation Group**, type Evaluation Group: Charge Efficiency in the **Label** text field.

Cumulative Amount of Salt Entering the Cell

- 1 In the **Evaluation Group: Charge Efficiency** toolbar, click  **Global Evaluation**.
- 2 In the **Settings** window for **Global Evaluation**, type Cumulative Amount of Salt Entering the Cell in the **Label** text field.


3 Locate the **Expressions** section. In the table, enter the following settings:

Expression	Unit	Description
Q*c_NaCl	mol/s	Inlet molar flow

4 Locate the **Data Series Operation** section. From the **Transformation** list, choose **Integral**.

5 Select the **Cumulative** checkbox.


Evaluation Group: Charge Efficiency

In the **Evaluation Group: Charge Efficiency** toolbar, click  **Integration** and choose **Line Integration**.

Cumulative Amount of Salt Exiting the Cell

1 In the **Settings** window for **Line Integration**, type Cumulative Amount of Salt Exiting the Cell in the **Label** text field.

2 Select Boundary 14 only.

3 Locate the **Expressions** section. Click  **Clear Table**.


4 In the table, enter the following settings:

Expression	Unit	Description
tcd.ntflux_cClm*d_z	mol/s	Outlet molar flow

5 Locate the **Data Series Operation** section. From the **Transformation** list, choose **Integral**.

6 Select the **Cumulative** checkbox.


Evaluation Group: Charge Efficiency

In the **Evaluation Group: Charge Efficiency** toolbar, click  **Integration** and choose **Line Integration**.

Cumulative Charge

1 In the **Settings** window for **Line Integration**, type Cumulative Charge in the **Label** text field.

2 Select Boundary 9 only.

3 Locate the **Expressions** section. Click  **Clear Table**.


4 In the table, enter the following settings:

Expression	Unit	Description
tcd.nIs*d_z	A	Boundary current

5 Locate the **Data Series Operation** section. From the **Transformation** list, choose **Integral**.

6 Select the **Cumulative** checkbox.

Evaluation Group: Charge Efficiency

- 1 In the **Model Builder** window, click **Evaluation Group: Charge Efficiency**.
- 2 In the **Settings** window for **Evaluation Group**, locate the **Transformation** section.
- 3 From the **Transformation type** list, choose **General**.
- 4 In the **Expression** text field, type $-(\text{gev1} - \text{int1}) * F_{\text{const}} / \text{int2} * 100$.
- 5 In the **Column header** text field, type Charge Efficiency.
- 6 In the **Evaluation Group: Charge Efficiency** toolbar, click  **Evaluate**.

EVALUATION GROUP: CHARGE EFFICIENCY

- 1 Go to the **Evaluation Group: Charge Efficiency** window.
- 2 Click the **Table Graph** button in the window toolbar.

RESULTS

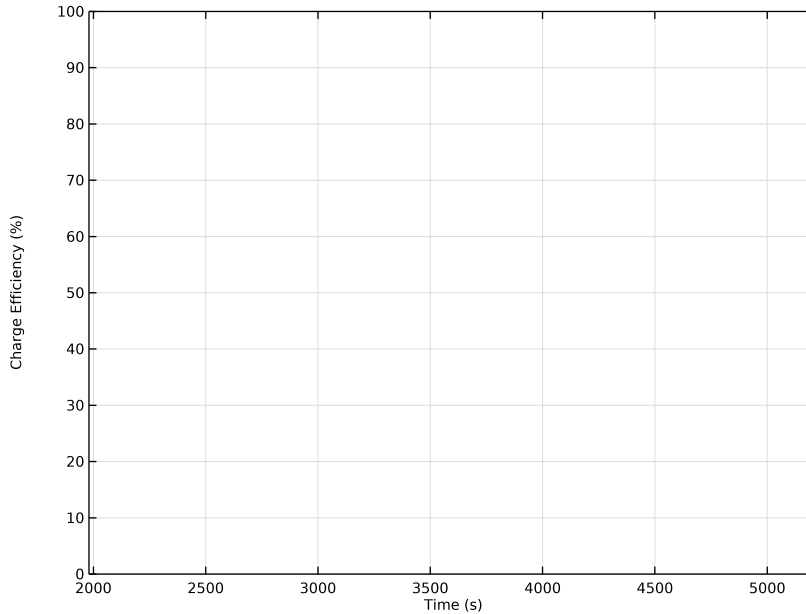
Table Graph 1

- 1 In the **Settings** window for **Table Graph**, locate the **Data** section.
- 2 From the **x-axis data** list, choose **Time (s)**.
- 3 From the **Plot columns** list, choose **Manual**.
- 4 In the **Columns** list box, select **Charge Efficiency (1)**.


Charge Efficiency

- 1 In the **Model Builder** window, under **Results** click **ID Plot Group 17**.
- 2 In the **Settings** window for **ID Plot Group**, type Charge Efficiency in the **Label** text field.
- 3 Locate the **Plot Settings** section.
- 4 Select the **y-axis label** checkbox. In the associated text field, type Charge Efficiency (%).
- 5 Locate the **Axis** section. Select the **Manual axis limits** checkbox.
- 6 In the **x minimum** text field, type 1980.
- 7 In the **x maximum** text field, type 5220.
- 8 In the **y minimum** text field, type 0.
- 9 In the **y maximum** text field, type 100.

10 In the **Charge Efficiency** toolbar, click  **Plot**.



Amount of Cl⁻ Stored in Micropores

- 1** In the **Results** toolbar, click  **ID Plot Group**.
- 2** In the **Settings** window for **ID Plot Group**, type Amount of Cl⁻ Stored in Micropores in the **Label** text field.
- 3** Locate the **Title** section. From the **Title type** list, choose **None**.
- 4** Locate the **Plot Settings** section.
- 5** Select the **x-axis label** checkbox. In the associated text field, type Time (s).
- 6** Select the **y-axis label** checkbox. In the associated text field, type Amount of Cl⁻ stored in micropores (μmol).
- 7** Select the **Two y-axes** checkbox.
- 8** Select the **Secondary y-axis label** checkbox. In the associated text field, type Applied potential (V).
- 9** Locate the **Legend** section. From the **Layout** list, choose **Outside graph axis area**.
- 10** From the **Position** list, choose **Bottom**.

Applied Potential


- 1** In the **Amount of Cl⁻ Stored in Micropores** toolbar, click  **Global**.

- 2 In the **Settings** window for **Global**, type Applied Potential in the **Label** text field.
- 3 Locate the **y-Axis** section. Select the **Plot on secondary y-axis** checkbox.
- 4 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component I (comp1) > Tertiary Current Distribution, Nernst-Planck > Load Cycle I > tcd.lcl.E_app - Applied voltage - V**.

Amount of Cl- Stored in Micropores

In the **Amount of Cl- Stored in Micropores** toolbar, click  **Global**.

Amount Stored

- 1 In the **Settings** window for **Global**, type Amount Stored in the **Label** text field.
- 2 Locate the **y-Axis Data** section. Click  **Clear Table**.
- 3 In the table, enter the following settings:

Expression	Unit	Description
n_Clm_upper	umol	Upper electrode
n_Clm_lower	umol	Lower electrode

- 4 In the **Amount of Cl- Stored in Micropores** toolbar, click  **Plot**.

