



Desalination in an Electrodialysis Cell

Introduction

Electrodialysis is a separation process for electrolytes based on the use of electric fields and ion selective membranes. Some common applications of the electrodialysis process are:

- Desalination of process streams, effluents, and drinking water
- pH regulation in order to remove acids from, for example, fruit juices and wines
- Metal electrowinning of precious metals

This tutorial demonstrates the basics of electrodialysis in a desalination cell.

Model Definition

Figure 1 shows the basic principle of the desalination stack. The stack has one repetitive cell unit, shown in Figure 2.

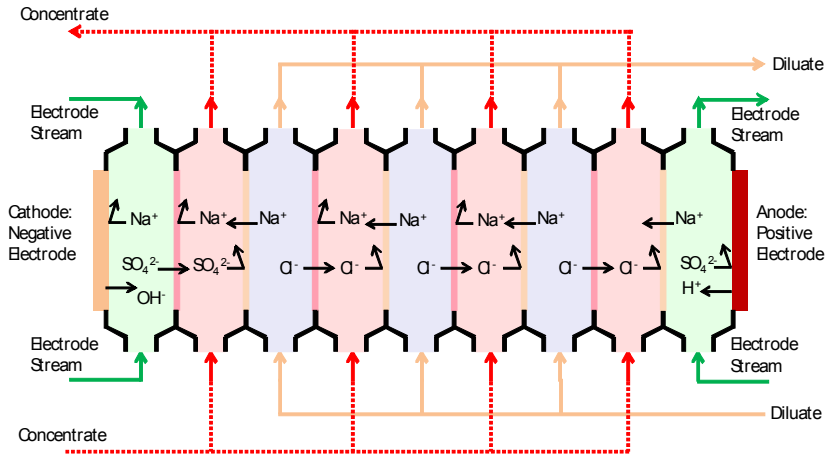


Figure 1: Schematic picture of a desalination stack with 3 desalination units (in reality 10 - 20 unit cells are used)

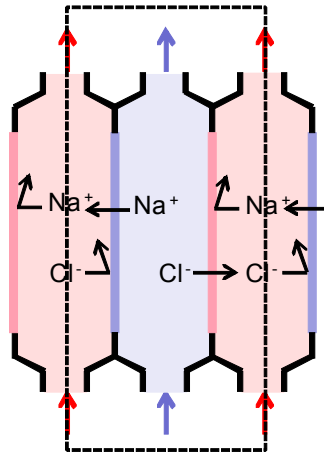


Figure 2: The repetitive unit cell with one desalination unit.

The model geometry for this example is based on the repetitive unit, excluding the inlet and outlet flow regions. The model geometry is shown in [Figure 3](#).

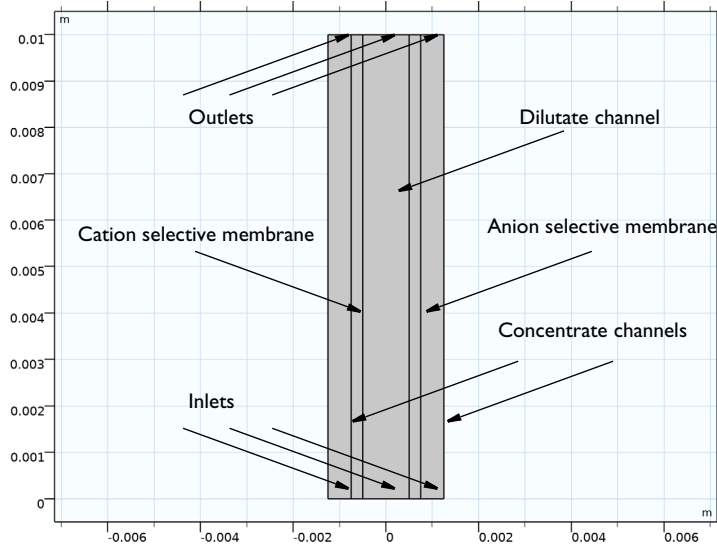


Figure 3: Model geometry.

The cell contains two ion selective membrane domains: the left is mainly permeable to cations, and the right to anions. The middle domain is a free flowing electrolyte domain, where salt is to be removed. This domain is named the dilute domain. The rightmost and leftmost domains are free flowing electrolyte domains, where the ion concentration increases during cell operation. These domains are called the concentrate domains. In the free electrolyte domains, the flow enters at the bottom inlets and exits at the top outlets at an average flow rate is $5 \text{ mm}\cdot\text{s}^{-1}$. An analytical expression (Poiseuille flow) for the fluid velocity is used in this model.

The cell is fed with a seawater electrolyte consisting of 0.5 M NaCl and operated at a unit cell voltage of 1.5 V .

CHOICE OF CURRENT DISTRIBUTION INTERFACE

In this model we make use of the Nernst-Planck equations for ion flux and charge transport by which the following equation describes the molar flux of species i (which is either Cl or Na in this model), \mathbf{N}_i , due to diffusion, migration and convection:

$$\mathbf{N}_i = -D_i \nabla c_i - z_i u_{\text{mob}, i} F c_i \nabla \phi_l + c_i \mathbf{u}$$

The first term is the diffusion flux, D_i is the diffusion coefficient (SI unit: m^2/s). The migration term consists of the species charge number z_i , the species mobility $u_{\text{mob},i}$ (SI unit: $\text{s}\cdot\text{mol}/\text{kg}$) and the electrolyte potential (ϕ_l). In the convection term, \mathbf{u} denotes the fluid velocity vector (SI unit: m/s).

The electrolyte current density is calculated using Faraday's law by summing up the contributions from the molar fluxes, multiplied by the species charges, with the observation that the convective term vanishes due to the electroneutrality condition (see the theory for the Tertiary Current Distribution, Nernst-Planck interface):

$$\mathbf{i}_l = F \sum_{i=1}^n z_i (-D_i \nabla c_i - z_i u_{\text{mob},i} F c_i \nabla \phi_l) \quad (1)$$

The conservation of current is then used to calculate the electrolyte potential.

$$\nabla \cdot \mathbf{i}_l = 0$$

This model uses Tertiary Current Distribution, Nernst-Planck interface when solving for the electrolyte potential in the free electrolyte and ion-selective membrane domains.

In the free electrolyte domains, the only ions present are assumed to be Na^+ and Cl^- . The ion selective membranes also contain additional ions fixed in a matrix. Therefore, the fixed space charge, ρ_{fix} , is added while calculating the sum of charges in the electroneutrality condition:

$$\rho_{\text{fix}} + F \sum_{i=1}^n z_i c_i = 0 \quad (2)$$

The fixed space charge is prescribed in terms of the membrane charge concentration which is varied using an auxiliary sweep in this model.

Note that the ion-selective membrane domains do allow for transport of both Na^+ and Cl^- but that the sign and magnitude of the fixed charge, in combination with the Donnan boundary conditions (described in the next section) will favor transport of either anions or cations. The sign of the fixed membrane charge is positive in the anion, and negative in the cation exchange membrane domains, respectively.

MEMBRANE — FREE ELECTROLYTE BOUNDARY CONDITIONS

The boundary conditions at the boundaries between the membrane and free electrolyte domains are set up in the following way:

The normal electrolyte current density is equal to the current density in the membrane:

$$\mathbf{n} \cdot \mathbf{i}_{l,e} = \mathbf{n} \cdot \mathbf{i}_{l,m} \quad (3)$$

The ion flux for each species is continuous over the membrane-free electrolyte interface:

$$\mathbf{n} \cdot \mathbf{N}_{i,e} = \mathbf{n} \cdot \mathbf{N}_{i,m} \quad (4)$$

Furthermore, we have the following relation between the potentials and the concentrations:

$$\phi_{l,m} = \phi_{l,e} - \frac{RT}{z_i F} \ln\left(\frac{c_{i,m}}{c_{i,e}}\right) \quad (5)$$

where $c_{i,m}$ is the species concentration in the membrane, and $c_{i,e}$ the species concentration in the free electrolyte and z_i the corresponding charge. The potential shift caused by Equation 5 is called Donnan potential, or dialysis potential.

Equation 3, Equation 4, and Equation 5 above represent a mix of Dirichlet and Neumann conditions for the electrolyte potential and species concentrations. The Ion Exchange Membrane domain feature in the Tertiary Current Distribution, Nernst-Planck interface is used to define these conditions.

PERIODIC CONDITION

Use the Periodic Condition feature to set the concentration on the rightmost boundary to equal that of the leftmost boundary and to set the electrolyte potential offset between the rightmost and leftmost boundaries.

USE OF AN AUXILIARY SWEEP TO FACILITATE CONVERGENCE

The model is solved using a Stationary study with an Auxiliary sweep, ramping up and solving for three different membrane charge concentrations: 0, 500, and 1000 mol/m³, iteratively using the previous solution for the lower concentration as initial values for the next concentration value.

Results and Discussion

Figure 4 shows the Na⁺ ion concentration in the cell for the membrane charge concentration of 1000 mol/m³. The concentration increases in the concentrate domains, and decreases in the dilutate domain. A boundary layer with high concentration gradients forms close to the membrane surfaces. In a real desalination cell it is common to add

spacers that, apart from adding mechanical stability to the cell, also induce convective mass transport in the direction perpendicular to the main flow, and hence may reduce the thickness of the boundary layer.

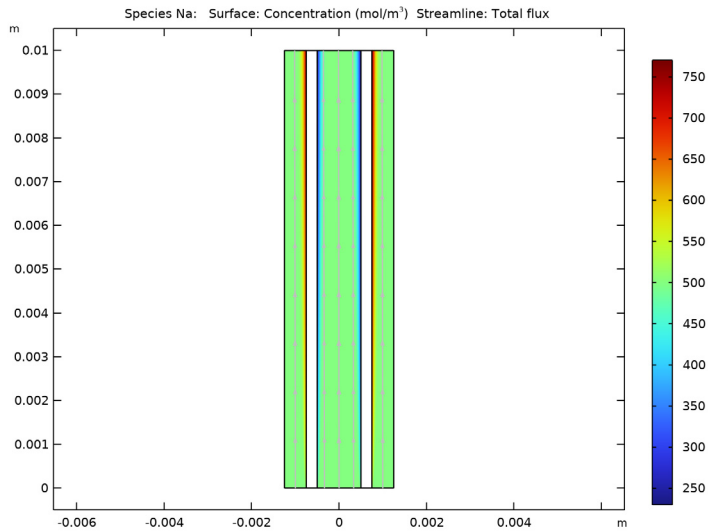


Figure 4: Ion concentration.

Figure 5 shows the electrolyte potential along a horizontal line placed at half the cell height. The main part of the potential losses occurs in the membranes. The Donnan potential discontinuity can be seen at the boundaries between the free electrolyte and membrane domains.

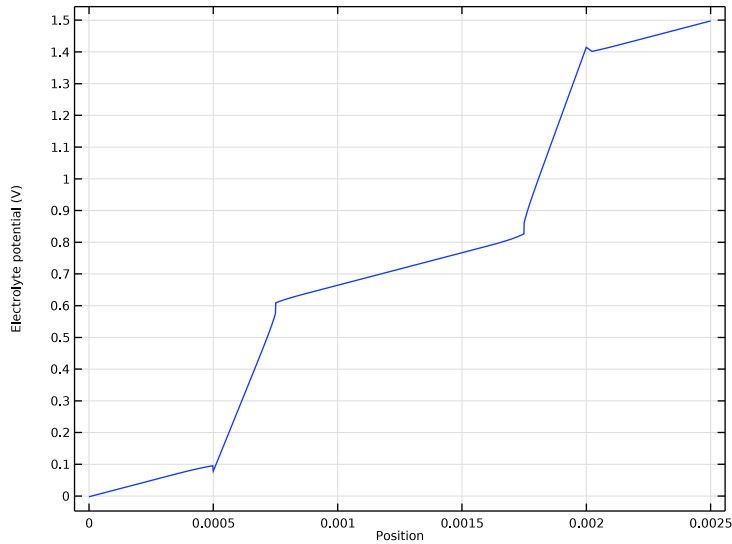


Figure 5: Electrolyte potential at half the cell height.

Figure 6 shows the concentration of Na^+ and Cl^- ions at half the cell height for the membrane charge concentration, 1000 mol/m^3 . The concentration of both Na^+ and Cl^- ions is higher in the concentrate domains and lower in the dilute domain, as also shown

in Figure 4. The concentration of Na^+ is significantly lower than for Cl^- in the anion-selective domain (and vice versa), but it is not zero.

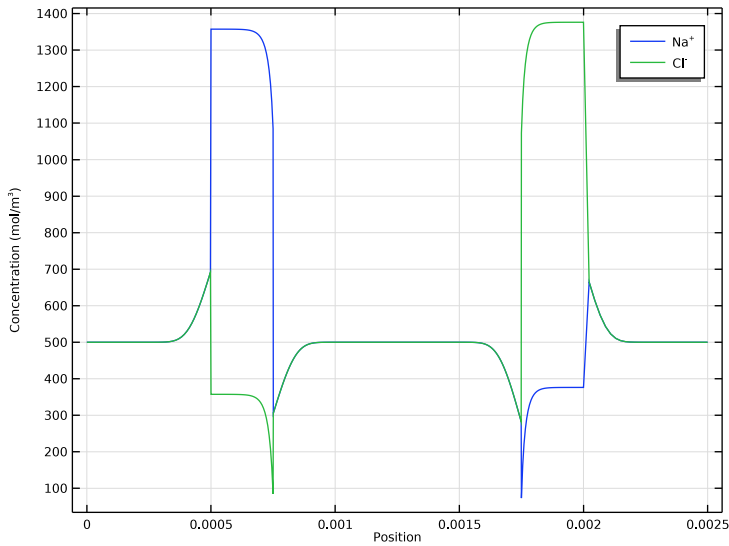


Figure 6: Ion concentrations at half the cell height for a membrane charge concentration of 1000 mol/m^3 .

Figure 7 and Figure 8 show a comparison between the migrative and diffusive fluxes in the free electrolyte for Na^+ and Cl^- , respectively. The diffusive fluxes get prominent close to the membrane boundaries due to the high concentration gradients. The migrative fluxes govern in the middle of the channels and have different signs for Na^+ and Cl^- due to the different signs of the ion charges.

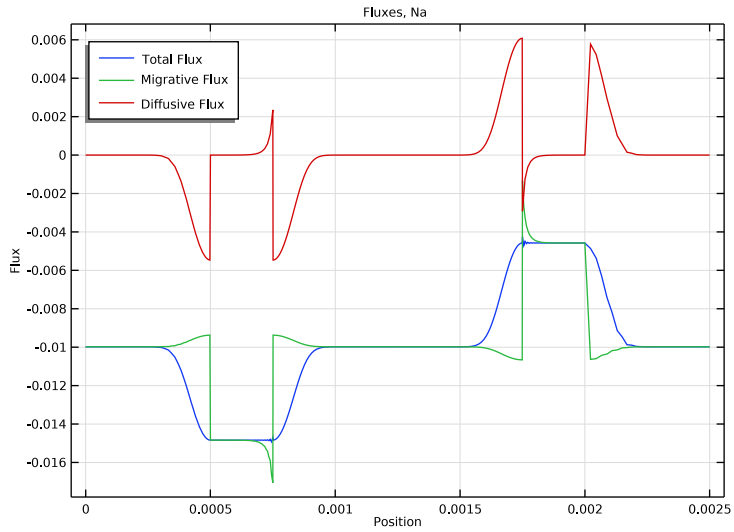


Figure 7: Comparison of fluxes, species Na^+ .

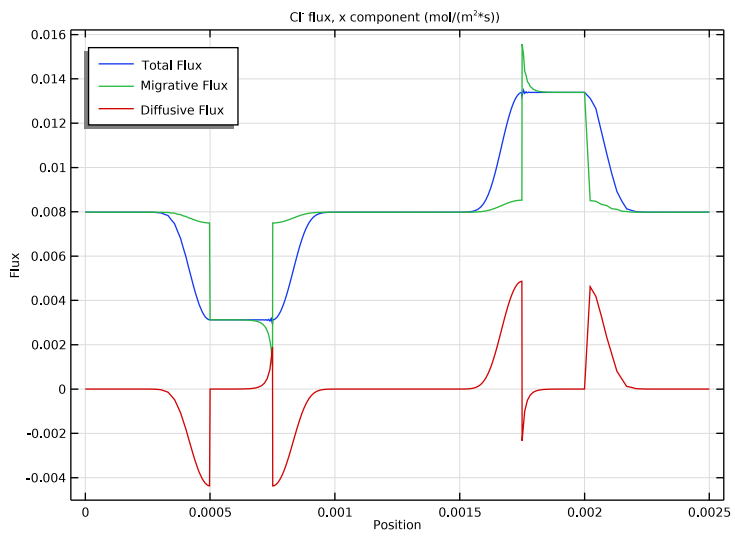


Figure 8: Comparison of fluxes, species Cl^- .

Finally, [Figure 9](#) shows the current density along the left free electrolyte–membrane boundary of the anion selective membrane for three different membrane charge concentrations: 0, 500, and 1000 mol/m³. Depletion of chloride gets more prominent toward the top of the cell, resulting in a higher Donnan potential shift and a higher negative current density.

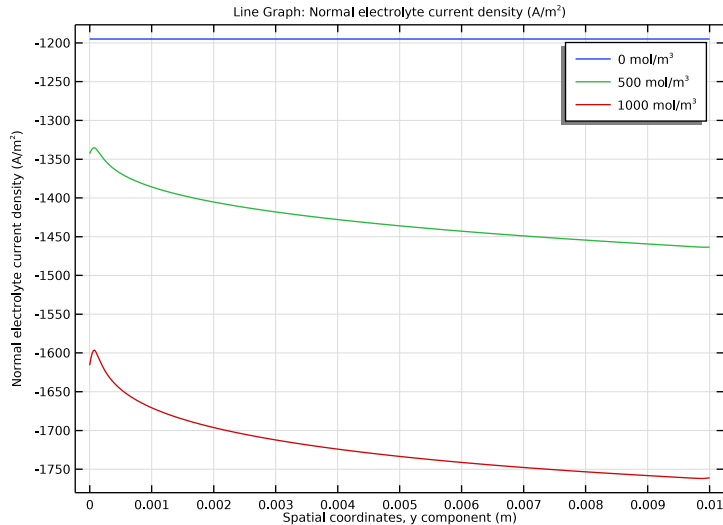



Figure 9: Normal current density along the membrane – free electrolyte boundary for the anion selective membrane for three different membrane charge concentrations, 0, 500, and 1000 mol/m³.

Application Library path: Electrochemistry_Module /
Electrochemical_Engineering/electrodialysis


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** table, enter the following settings:

cNa
cCl
- 5 Click  **Study**.
- 6 In the **Select Study** tree, select **General Studies>Stationary**.
- 7 Click  **Done**.

GLOBAL DEFINITIONS

Parameters 1



Load the model parameters from a text file.

- 1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.
- 2 In the **Settings** window for **Parameters**, locate the **Parameters** section.
- 3 Click  **Load from File**.
- 4 Browse to the model's Application Libraries folder and double-click the file `electrodialysis_parameters.txt`.

GEOMETRY 1


Draw the geometry as a set of rectangles.

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 $2 \cdot (W_{ch} + W_m)$.
- 4 In the **Height** text field, type L .
- 5 Locate the **Position** section. In the **x** text field, type $-(W_{ch} + W_m)$.
- 6 Click  **Build Selected**.

Rectangle 2 (r2)

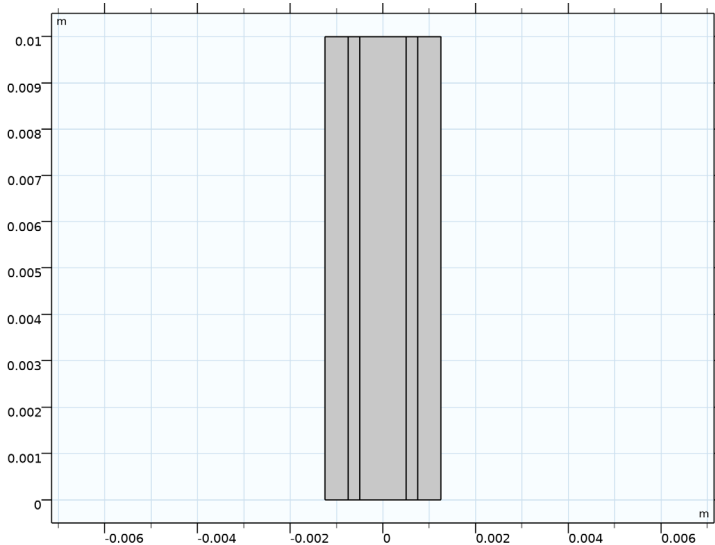
- 1 In the **Geometry** toolbar, click  **Rectangle**.

- 2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
- 3 In the **Width** text field, type $(W_{ch}+2*W_m)$.
- 4 In the **Height** text field, type L .
- 5 Locate the **Position** section. In the **x** text field, type $-(W_{ch}+2*W_m)/2$.
- 6 Click  **Build Selected**.

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 W_{ch} .
- 4 In the **Height** text field, type L .
- 5 Locate the **Position** section. In the **x** text field, type $-W_{ch}/2$.
- 6 Click  **Build Selected**.
- 7 Click the  **Zoom Extents** button in the **Graphics** toolbar.

The finished geometry should look like the figure below.



DEFINITIONS

Make some selections on the geometry to use later when you set up the physics.

Membrane (Cation Selective)

- 1 In the **Definitions** toolbar, click  **Explicit**.

2 In the **Settings** window for **Explicit**, type Membrane (Cation Selective) in the **Label** text field.

3 Select Domain 2 only.

Membrane (Anion Selective)

1 In the **Definitions** toolbar, click  **Explicit**.

2 In the **Settings** window for **Explicit**, type Membrane (Anion Selective) in the **Label** text field.

3 Select Domain 4 only.

Channels

1 In the **Definitions** toolbar, click  **Explicit**.

2 In the **Settings** window for **Explicit**, type Channels in the **Label** text field.

3 Select Domains 1, 3, and 5 only.

Inlets

1 In the **Definitions** toolbar, click  **Explicit**.

2 In the **Settings** window for **Explicit**, type Inlets in the **Label** text field.

3 Locate the **Input Entities** section. From the **Geometric entity level** list, choose **Boundary**.

4 Select Boundaries 2, 8, and 14 only.

Outlets

1 In the **Definitions** toolbar, click  **Explicit**.

2 In the **Settings** window for **Explicit**, type Outlets in the **Label** text field.

3 Locate the **Input Entities** section. From the **Geometric entity level** list, choose **Boundary**.

4 Select Boundaries 3, 9, and 15 only.

Analytic 1 (an1)

Define an analytical function to account for the convectonal velocity for the different domains.

1 In the **Definitions** toolbar, click  **Analytic**.

2 In the **Settings** window for **Analytic**, type ve1 in the **Function name** text field.

3 Locate the **Definition** section. In the **Expression** text field, type $3*v_avg*(1 - ((t)/(W_ch/2))^2)$.

4 In the **Arguments** text field, type t .

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

Argument	Unit
t	m

6 In the **Function** text field, type m/s.

7 Locate the **Plot Parameters** section. In the table, enter the following settings:

Argument	Lower limit	Upper limit	Unit
t	-1	1	m

Variables 1

Now add some variables to the model. Use the predefined analytic function **vel** to define the velocity variable across different channels.

- 1 In the **Definitions** toolbar, click **a= Local Variables**.
- 2 In the **Settings** window for **Variables**, locate the **Geometric Entity Selection** section.
- 3 From the **Geometric entity level** list, choose **Domain**.
- 4 Select Domain 3 only.
- 5 Locate the **Variables** section. In the table, enter the following settings:

Name	Expression	Unit	Description
vel	vel(x)	m/s	Channel velocity (middle channel)

Variables 2

- 1 In the **Definitions** toolbar, click **a= Local Variables**.
- 2 In the **Settings** window for **Variables**, locate the **Geometric Entity Selection** section.
- 3 From the **Geometric entity level** list, choose **Domain**.
- 4 Select Domain 1 only.
- 5 Locate the **Variables** section. In the table, enter the following settings:

Name	Expression	Unit	Description
vel	vel((x+W_ch+W_m))	m/s	Channel velocity (left channel)

Variables 3

- 1 In the **Definitions** toolbar, click **a= Local Variables**.
- 2 In the **Settings** window for **Variables**, locate the **Geometric Entity Selection** section.
- 3 From the **Geometric entity level** list, choose **Domain**.

4 Select Domain 5 only.

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

Name	Expression	Unit	Description
vel	$vel(x-W_{ch}-W_m)$	m/s	Channel velocity (right channel)

TERTIARY CURRENT DISTRIBUTION, NERNST-PLANCK (TCD)

Now, start setting up the physics, start with the free electrolyte channels.

Electrolyte 1

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

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

3 Specify the **u** vector as

0	x
vel	y

4 Locate the **Diffusion** section. In the D_{cNa} text field, type DNA.

5 In the D_{cCl} text field, type DC1.

6 Locate the **Migration in Electric Field** section. In the z_{cNa} text field, type 1.

7 In the z_{cCl} text field, type -1.

Ion Exchange Membrane (Cation Selective)

Use the Ion Exchange Membrane domain feature to solve for the electrolyte potential and concentrations in the cation selective membrane domain. The electrolyte potential and concentrations in the membrane and free electrolyte domains is coupled by applying Donnan potential expression on the boundaries between them.

1 In the **Physics** toolbar, click  **Domains** and choose **Ion Exchange Membrane**.

2 In the **Settings** window for **Ion Exchange Membrane**, type Ion Exchange Membrane (Cation Selective) in the **Label** text field.

3 Locate the **Domain Selection** section. From the **Selection** list, choose **Membrane (Cation Selective)**.

4 Locate the **Ion Exchange Membrane Properties** section. In the ρ_{fix} text field, type $-cMem * F_{const}$.

5 Locate the **Diffusion** section. In the D_{cNa} text field, type DNA.

- 6 In the D_{cCl} text field, type DC1.
- 7 Locate the **Migration in Electric Field** section. In the z_{cNa} text field, type 1.
- 8 In the z_{cCl} text field, type -1.
- 9 Locate the **Porous Matrix Properties** section. In the ϵ_1 text field, type 0.15.


Ion Exchange Membrane (Anion Selective)

Similarly, use the Ion Exchange Membrane domain feature to set the anion selective membrane.

- 1 Right-click **Ion Exchange Membrane (Cation Selective)** and choose **Duplicate**.
- 2 In the **Settings** window for **Ion Exchange Membrane**, type Ion Exchange Membrane (Anion Selective) in the **Label** text field.
- 3 Locate the **Domain Selection** section. From the **Selection** list, choose **Membrane (Anion Selective)**.
- 4 Locate the **Ion Exchange Membrane Properties** section. In the ρ_{fix} text field, type $cMem^* F_{const}$.

Periodic Condition 1

Now, use the periodic condition feature to set the concentration on the rightmost boundary to be equal its corresponding value on the leftmost boundary and to set the electrolyte potential offset between the two boundaries.


- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Periodic Condition**.
- 2 Select Boundaries 1 and 16 only.
- 3 In the **Settings** window for **Periodic Condition**, locate the **Periodic Condition** section.
- 4 In the $\phi_{1,src} - \phi_{1,dst}$ text field, type $-V_{tot}$.
- 5 Clear the **Apply for electrode phase** check box.

Electrolyte Potential 1

Also, bootstrap the electrolyte potential using the point feature.


- 1 In the **Physics** toolbar, click  **Points** and choose **Electrolyte Potential**.
- 2 Select Point 1 only.

Inflow 1

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Inflow**.
- 2 In the **Settings** window for **Inflow**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Inlets**.
- 4 Locate the **Concentration** section. In the $c_{0,cCl}$ text field, type cCl_0 .

- 5 Locate the **Boundary Condition Type** section. From the list, choose **Flux (Danckwerts)**.

Outflow 1

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Outflow**.
- 2 In the **Settings** window for **Outflow**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Outlets**.

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 *cCl* text field, type *cCl_0*.
- 4 In the *phil* text field, type $V_{tot} * x / L$.

GLOBAL DEFINITIONS

Default Model Inputs


Set up the temperature value used in the entire model.

- 1 In the **Model Builder** window, under **Global Definitions** click **Default Model Inputs**.
- 2 In the **Settings** window for **Default Model Inputs**, locate the **Browse Model Inputs** section.
- 3 In the tree, select **General>Temperature (K) - minput.T**.
- 4 Find the **Expression for remaining selection** subsection. In the **Temperature** text field, type *T*.

MESH 1

The physics settings are now complete. A mapped mesh is suitable for this geometry. Use distributions to obtain thinner elements in the free electrolyte close to the membrane surfaces.


Mapped 1

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


Distribution 1

- 1 Right-click **Mapped 1** and choose **Distribution**.
- 2 Select Boundary 1 only.
- 3 In the **Settings** window for **Distribution**, locate the **Distribution** section.
- 4 In the **Number of elements** text field, type 100.


Distribution 2

- 1 Right-click **Distribution 1** and choose **Duplicate**.
- 2 In the **Settings** window for **Distribution**, locate the **Boundary Selection** section.
- 3 Click  **Clear Selection**.
- 4 Select Boundaries 8 and 9 only.
- 5 Locate the **Distribution** section. From the **Distribution type** list, choose **Predefined**.
- 6 In the **Number of elements** text field, type 100.
- 7 In the **Element ratio** text field, type 10.
- 8 Select the **Symmetric distribution** check box.


Distribution 3

- 1 Right-click **Distribution 2** and choose **Duplicate**.
- 2 In the **Settings** window for **Distribution**, locate the **Boundary Selection** section.
- 3 Click  **Clear Selection**.
- 4 Select Boundaries 3 and 14 only.
- 5 Locate the **Distribution** section. In the **Number of elements** text field, type 20.
- 6 Clear the **Symmetric distribution** check box.
- 7 Select the **Reverse direction** check box.

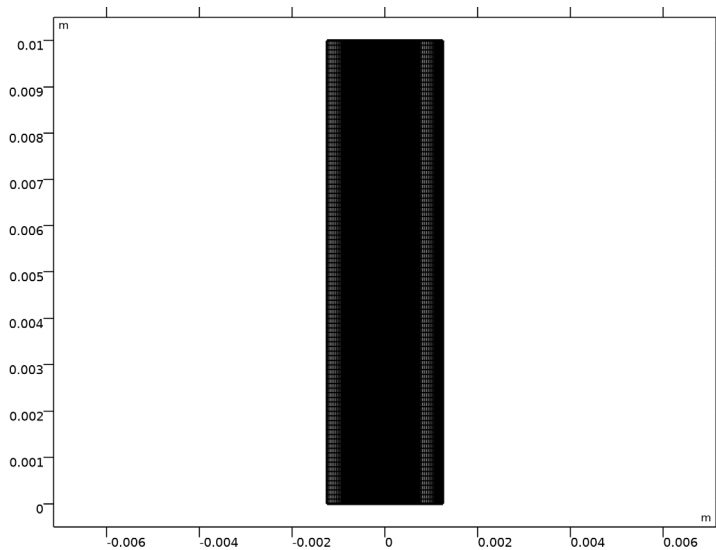
Distribution 4

- 1 Right-click **Distribution 3** and choose **Duplicate**.
- 2 In the **Settings** window for **Distribution**, locate the **Boundary Selection** section.
- 3 Click  **Clear Selection**.
- 4 Select Boundaries 2 and 15 only.
- 5 Locate the **Distribution** section. Clear the **Reverse direction** check box.

Distribution 5

- 1 Right-click **Distribution 4** and choose **Duplicate**.
- 2 In the **Settings** window for **Distribution**, locate the **Boundary Selection** section.
- 3 Click  **Clear Selection**.
- 4 Select Boundaries 6 and 12 only.
- 5 Locate the **Distribution** section. In the **Element ratio** text field, type 2.
- 6 Select the **Symmetric distribution** check box.

- 7** In the **Model Builder** window, right-click **Mesh 1** and choose **Build All**.
After completion the mesh should resemble the figure below.



STUDY 1

Step 1: Stationary


The problem is now ready for solving. Use an auxiliary sweep to solve for a range of membrane charge concentration.

- 1** In the **Model Builder** window, under **Study 1** click **Step 1: Stationary**.
- 2** In the **Settings** window for **Stationary**, click to expand the **Study Extensions** section.
- 3** Select the **Auxiliary sweep** check box.
- 4** Click **+ Add**.
- 5** In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
cMem (Membrane charge concentration)	0 500 1000	mol/m ³

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, under **Study 1 > Solver Configurations > Solution 1 (sol1)** click **Stationary Solver 1**.
- 4 In the **Settings** window for **Stationary Solver**, locate the **General** section.
- 5 In the **Relative tolerance** text field, type $1e-5$.
- 6 In the **Study** toolbar, click  **Compute**.


RESULTS

Concentration, Na (tcd)


Reproduce the figures from the [Results and Discussion](#) section in the following way.

- 1 In the **Model Builder** window, under **Results** click **Concentration, Na (tcd)**.
- 2 In the **Settings** window for **2D Plot Group**, click to expand the **Selection** section.
- 3 From the **Geometric entity level** list, choose **Domain**.
- 4 From the **Selection** list, choose **Channels**.



Streamline 1

- 1 In the **Model Builder** window, expand the **Concentration, Na (tcd)** node, then 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 5.
- 5 Locate the **Selection** section. Click to select the  **Activate Selection** toggle button.
- 6 From the **Selection** list, choose **Inlets**.


Concentration, Na (tcd)

- 1 In the **Model Builder** window, click **Concentration, Na (tcd)**.
- 2 In the **Settings** window for **2D Plot Group**, click to expand the **Title** section.
- 3 Find the **Solution** subsection. Clear the **Solution** check box.
- 4 In the **Concentration, Na (tcd)** toolbar, click  **Plot**.



Cut Line 2D 1

- 1 In the **Results** toolbar, click  **Cut Line 2D**.
- 2 In the **Settings** window for **Cut Line 2D**, locate the **Line Data** section.
- 3 In row **Point 1**, set **X** to $-W_{ch}-W_m$ and **y** to $L/2$.
- 4 In row **Point 2**, set **X** to $W_{ch}+W_m$ and **y** to $L/2$.
- 5 Click  **Plot**.


Potential

- 1 In the **Results** toolbar, click  **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, type Potential in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Cut Line 2D I**.
- 4 From the **Parameter selection (cMem)** list, choose **Last**.
- 5 Click to expand the **Title** section. From the **Title type** list, choose **None**.
- 6 Locate the **Plot Settings** section. Select the **x-axis label** check box.
- 7 In the associated text field, type Position.


Line Graph I

- 1 In the **Potential** toolbar, click  **Line Graph**.
- 2 Click  **Plot**.

Concentrations

- 1 In the **Home** toolbar, click  **Add Plot Group** and choose **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, type Concentrations in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Cut Line 2D I**.
- 4 From the **Parameter selection (cMem)** list, choose **Last**.
- 5 Locate the **Title** section. From the **Title type** list, choose **None**.
- 6 Locate the **Plot Settings** section. Select the **x-axis label** check box.
- 7 In the associated text field, type Position.

Line Graph I

- 1 In the **Concentrations** toolbar, click  **Line Graph**.
- 2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
- 3 In the **Expression** text field, type cNa.
- 4 Click to expand the **Legends** section. Select the **Show legends** check box.
- 5 From the **Legends** list, choose **Manual**.
- 6 In the table, enter the following settings:


Legends

Na[⁺]

Concentrations


In the **Model Builder** window, click **Concentrations**.

Line Graph 2


- 1 In the **Concentrations** toolbar, click  **Line Graph**.
- 2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
- 3 In the **Expression** text field, type `cCl`.
- 4 Locate the **Legends** section. Select the **Show legends** check box.
- 5 From the **Legends** list, choose **Manual**.
- 6 In the table, enter the following settings:

Legends


`cCl>`

- 7 In the **Concentrations** toolbar, click  **Plot**.

Fluxes, Na

- 1 In the **Home** toolbar, click  **Add Plot Group** and choose **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, type `Fluxes, Na` in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Cut Line 2D I**.
- 4 From the **Parameter selection (cMem)** list, choose **Last**.

Line Graph 1

- 1 In the **Fluxes, Na** toolbar, click  **Line Graph**.
- 2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
- 3 In the **Expression** text field, type `tcd.tflux_cNa`.
- 4 Locate the **Legends** section. Select the **Show legends** check box.
- 5 From the **Legends** list, choose **Manual**.
- 6 In the table, enter the following settings:

Legends

`Total Flux`


Line Graph 2

- 1 Right-click **Line Graph 1** and choose **Duplicate**.
- 2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
- 3 In the **Expression** text field, type `tcd.mflux_cNax`.

4 Locate the **Legends** section. In the table, enter the following settings:


Legends
Migrative Flux

Line Graph 3

- 1 Right-click **Line Graph 2** and choose **Duplicate**.
- 2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
- 3 In the **Expression** text field, type `tcd.dflux_cNa`.
- 4 In the **Fluxes, Na** toolbar, click  **Plot**.
- 5 Locate the **Legends** section. In the table, enter the following settings:

Legends
Diffusive Flux

Fluxes, Na

- 1 In the **Model Builder** window, click **Fluxes, Na**.
- 2 In the **Settings** window for **ID Plot Group**, locate the **Plot Settings** section.
- 3 Select the **x-axis label** check box.
- 4 In the associated text field, type `Position`.
- 5 Select the **y-axis label** check box.
- 6 In the associated text field, type `Flux`.
- 7 Locate the **Title** section. From the **Title type** list, choose **Label**.
- 8 Locate the **Legend** section. From the **Position** list, choose **Upper left**.
- 9 In the **Fluxes, Na** toolbar, click  **Plot**.

Fluxes, Cl

- 1 Right-click **Fluxes, Na** and choose **Duplicate**.
- 2 In the **Settings** window for **ID Plot Group**, locate the **Title** section.
- 3 From the **Title type** list, choose **Manual**.
- 4 In the **Label** text field, type `Fluxes, Cl`.

Line Graph 1

- 1 In the **Model Builder** window, expand the **Fluxes, Cl** node, then click **Line Graph 1**.
- 2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
- 3 In the **Expression** text field, type `tcd.tfluxx_cCl`.


Line Graph 2

- 1 In the **Model Builder** window, click **Line Graph 2**.
- 2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
- 3 In the **Expression** text field, type `tcd.mflux_cClx`.


Line Graph 3

- 1 In the **Model Builder** window, click **Line Graph 3**.
- 2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
- 3 In the **Expression** text field, type `tcd.dflux_cClx`.




Fluxes, Cl

- 1 In the **Model Builder** window, click **Fluxes, Cl**.
- 2 In the **Settings** window for **ID Plot Group**, locate the **Title** section.
- 3 In the **Title** text area, type Cl^{flux} , x component ($\text{mol}/(\text{m}^2 \cdot \text{s})$).
- 4 In the **Fluxes, Cl** toolbar, click  **Plot**.

Electrolyte current density

- 1 In the **Home** toolbar, click  **Add Plot Group** and choose **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, type Electrolyte current density in the **Label** text field.

Line Graph 1

- 1 In the **Electrolyte current density** toolbar, click  **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 Boundary 10 only.
- 5 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.nll - Normal electrolyte current density - A/m²**.
- 6 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.
- 7 In the **Expression** text field, type `y`.
- 8 Locate the **Legends** section. Select the **Show legends** check box.
- 9 In the **Electrolyte current density** toolbar, click  **Plot**.

