

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 1shows 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 diluate 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 mm·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:

$$\mathbf{N}_{i} = -D_{i}\nabla c_{i} - z_{i}u_{\text{mob.}i}Fc_{i}\nabla\phi_{l} + c_{i}\mathbf{u}$$

The first term is the diffusion flux, D_i is the diffusion coefficient (SI unit: m²/s). The migration term consists of the species charge number z_i , the species mobility $u_{\text{mob},i}$ (SI unit: s·mol/kg) and the electrolyte potential (ϕ_l). In the convection term, **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):

$$\mathbf{i}_{l} = F \sum_{i=1}^{n} z_{i} (-D_{i} \nabla c_{i} - z_{i} u_{\mathbf{m}, i} F c_{i} \nabla \phi_{l})$$
(1)

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

$$\nabla \cdot \mathbf{i}_{1} = \mathbf{0}$$

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:

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

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:

$$\mathbf{n} \cdot \mathbf{i}_{l,e} = \mathbf{n} \cdot \mathbf{i}_{l,m} \tag{3}$$

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

$$\mathbf{n} \cdot \mathbf{N}_{i,e} = \mathbf{n} \cdot \mathbf{N}_{i,m} \tag{4}$$

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

$$\phi_{l,m} = \phi_{l,e} - \frac{RT}{z_i F} \ln\left(\frac{c_{i,m}}{c_{i,e}}\right)$$
(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/ m^3 , 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 diluate 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/m³. The concentration of both Na^+ and Cl^- ions is higher in the concentrate domains and lower in the diluate domain, as also shown

in Figure 4. The concentration of Na⁺ is significantly lower than for Cl⁻ in the anionselective 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⁻.

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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/ m^3 .

Application Library path: Electrochemistry_Module/ Electrochemical_Engineering/electrodialysis

Modeling Instructions

From the File menu, choose New.

NEW

In the New window, click Solution Model Wizard.

MODEL WIZARD

- I 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 \bigcirc Study.

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

7 Click M Done.

GLOBAL DEFINITIONS

Parameters 1

Load the model parameters from a text file.

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

Draw the geometry as a set of rectangles.

Rectangle 1 (r1)

- I 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*(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 틤 Build Selected.

Rectangle 2 (r2)

I 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 틤 Build Selected.

Rectangle 3 (r3)

- I 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 틤 Build Selected.
- 7 Click the $4 \rightarrow$ 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)

I 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)

- I 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

- I In the **Definitions** toolbar, click **here Explicit**.
- 2 In the Settings window for Explicit, type Channels in the Label text field.
- **3** Select Domains 1, 3, and 5 only.

Inlets

- I In the **Definitions** toolbar, click **here 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

- I 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 I (an I)

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

- I In the **Definitions** toolbar, click $\bigcap_{\alpha}^{f(\infty)}$ Analytic.
- 2 In the Settings window for Analytic, type vel 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 I

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

- I In the **Definitions** toolbar, click $\partial =$ **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

- I In the **Definitions** toolbar, click $\partial =$ **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	<pre>vel((x+W_ch+W_m))</pre>	m/s	Channel velocity (left channel)

Variables 3

- I In the **Definitions** toolbar, click $\partial =$ **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	<pre>vel((x-W_ch-W_m))</pre>	m/s	Channel velocity (right channel)

TERTIARY CURRENT DISTRIBUTION, NERNST-PLANCK (TCD)

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

Species Charges 1

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

Electrolyte I

- I In the Model Builder window, click Electrolyte I.
- 2 In the Settings window for Electrolyte, locate the Convection section.
- **3** Specify the **u** vector as

0	x
vel	у

- **4** Locate the **Diffusion** section. In the D_{cNa} text field, type DNa.
- **5** In the D_{cCl} text field, type DC1.

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.

- I 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 lon 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 $D_{\rm cCl}$ text field, type DC1.
- 7 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.

- I 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 lon Exchange Membrane Properties section. In the $\rho_{\rm fix}$ 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.

- I 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 $\phi_{l,src} \phi_{l,dst}$ text field, type Vtot.
- **5** Clear the **Apply for electrode phase** check box.

Electrolyte Potential I

Also, bootstrap the electrolyte potential using the point feature.

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

Inflow I

- I 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 I

- I 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

- I In the Model Builder window, click Initial Values I.
- 2 In the Settings window for Initial Values, locate the Initial Values section.
- **3** In the *cCl* text field, type cC1_0.
- **4** In the *phil* text field, type Vtot*x/L.

GLOBAL DEFINITIONS

Default Model Inputs

Set up the temperature value used in the entire model.

- I 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.
- Find the Expression for remaining selection subsection. In the Temperature text field, type T.

MESH I

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 I

- I Right-click Mapped I 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

- I Right-click Distribution I 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

- I 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

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

Distribution 5

- I 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 I and choose Build All.

0.01 0.009 0.008 0.007 0.006 0.005 0.004 0.003 0.002 0.001 0 6 -0.006 -0.004 -0.002 0.002 0.004 0.006

After completion the mesh should resemble the figure below.

STUDY I

Step 1: Stationary

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

- I In the Model Builder window, under Study I click Step I: 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	0 500 1000	mol/m^3
concentration)		

Solution 1 (soll)

- I In the Study toolbar, click **Show Default Solver**.
- 2 In the Model Builder window, expand the Solution I (soll) node.

- 3 In the Model Builder window, under Study I>Solver Configurations>Solution I (soll) click Stationary Solver I.
- 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.

- I 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

- I In the Model Builder window, expand the Concentration, Na (tcd) node, then click Streamline I.
- 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 **Delivate Selection** toggle button.
- 6 From the Selection list, choose Inlets.

Concentration, Na (tcd)

- I 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 **O Plot**.

Cut Line 2D I

- I In the **Results** toolbar, click \square **Cut Line 2D**.
- 2 In the Settings window for Cut Line 2D, locate the Line Data section.
- 3 In row Point I, 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

- I In the **Results** toolbar, click \sim **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.
- 7 Select the **x-axis label** check box. In the associated text field, type Position.

Line Graph I

- I In the Potential toolbar, click 📐 Line Graph.
- 2 Click 💿 Plot.

Concentrations

- I 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.
- 7 Select the x-axis label check box. In the associated text field, type Position.

Line Graph I

- I 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

- I In the Concentrations toolbar, click \sim Line Graph.
- 2 In the Settings window for Line Graph, locate the y-Axis Data section.
- **3** In the **Expression** text field, type cC1.
- 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

Cl⁻

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

Fluxes, Na

- I 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

- I 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.tfluxx_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

- I Right-click Line Graph I 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

- I 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_cNax.
- 4 In the Fluxes, Na toolbar, click **I** Plot.
- 5 Locate the Legends section. In the table, enter the following settings:

Legends

Diffusive Flux

Fluxes, Na

- I 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. In the associated text field, type **Position**.
- 4 Select the y-axis label check box. In the associated text field, type Flux.
- 5 Locate the Title section. From the Title type list, choose Label.
- 6 Locate the Legend section. From the Position list, choose Upper left.
- 7 In the Fluxes, Na toolbar, click 💽 Plot.

Fluxes, Cl

- I 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 I

- I In the Model Builder window, expand the Fluxes, Cl node, then click Line Graph I.
- 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

I 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

- I 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

- I 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 (mol/(m<sup>2</ sup>*s)).
- 4 In the Fluxes, CI toolbar, click 💿 Plot.

Electrolyte current density

- I 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 I

- I In the Electrolyte current density toolbar, click \sim Line Graph.
- 2 In the Settings window for Line Graph, locate the Selection section.
- **3** Click to select the **EXACTIVATE 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 I (compl)>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.

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