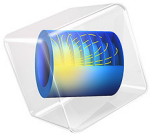


Isoelectric Separation

Introduction

This modeling example applies the Electrophoretic Transport and the Laminar Flow interfaces to model isoelectric separation in a free-flow electrophoresis device. A stream containing four different proteins is divided into separated component streams by means of migrative transport in an electric field.

Free flow electrophoresis can be used to separate macromolecules, such as proteins perpendicular to the flow of the carrier fluid. If a pH and potential gradient is applied across the carrier flow, then molecules can be focused along their isoelectric points. The isoelectric point is the pH at which a molecule has zero net charge. The concept of isoelectric focusing is illustrated in Figure 1.

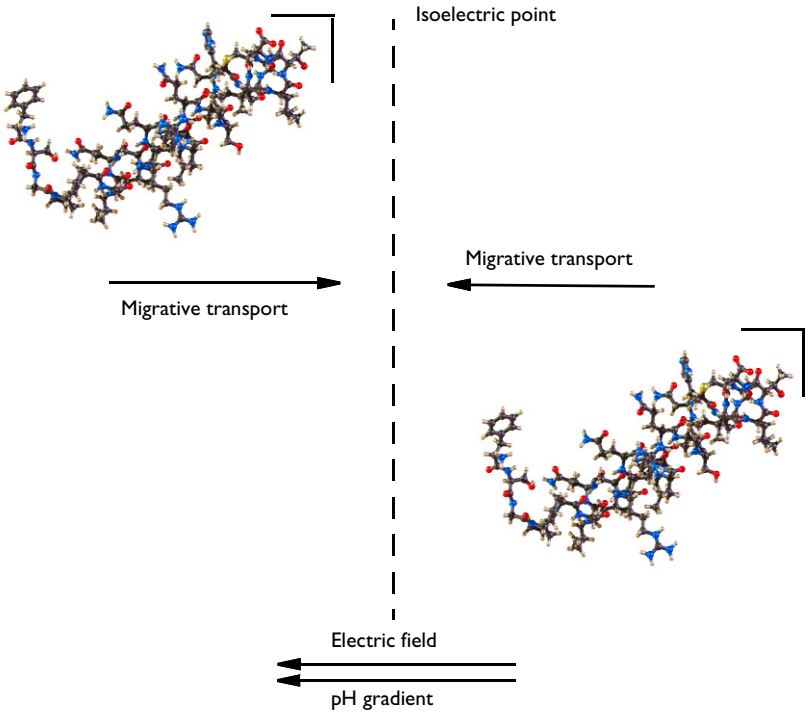


Figure 1: Ampholytic molecules can be focused around their isoelectric point by means of migrative transport in an electric field.

Molecules with a positive net charge travel in the direction of the electric field, along the pH gradient, until they reach the isoelectric point. At this instance the migrative transport

is switched off as the molecules net charge is zero. Similarly, negative net charge species travel in the direction opposite of the electric field.

Model Definition

The model geometry is shown in Figure 2. It represents the separation region in an isoelectric focusing chip. A laminar carrier stream transports a mixture of four proteins, one weak acid and one weak base, injected at the bottom of the cell.

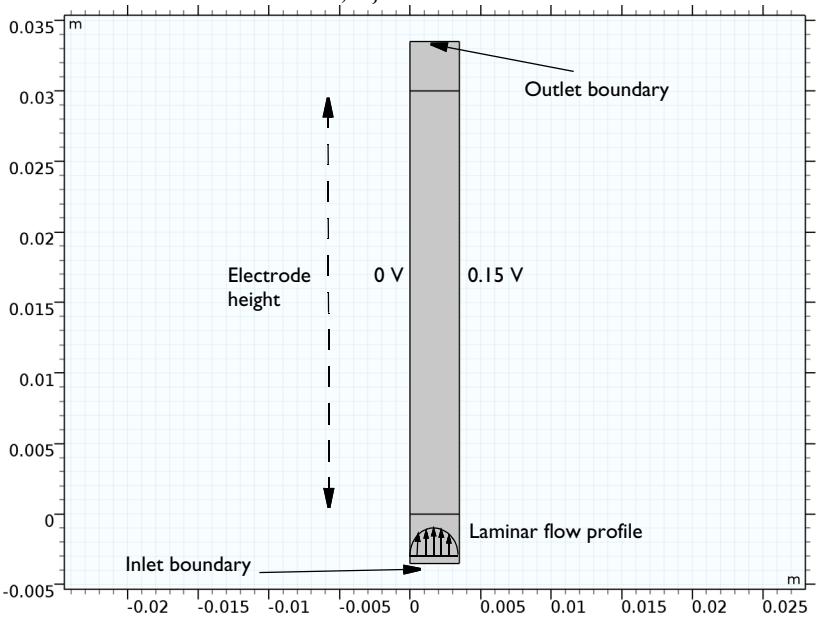


Figure 2: Model geometry.

The Electrophoretic Transport interface supports ionic species transport by diffusion, convection, and migration in electric fields. The mass balance that is solved in the interface is as follows:

$$\nabla \cdot (-D_i \nabla c_i - z_i u_{\mathrm{m},i} F c_i \nabla \phi) + \mathbf{u} \cdot \nabla c_i = 0$$

In the equation, c_i denotes the concentration of species i (SI unit: mol/m^3), D_i is the diffusion coefficient of species i (SI unit: m^2/s), $\mathbf{u}$ is the fluid velocity (SI unit: m/s), F refers to Faraday's constant (SI unit: s·A/mol), ϕ denotes the electric potential (SI unit: V), z_i is the charge number of the ionic species (unitless), and $u_{m,i}$ its ionic mobility (SI unit: s·mol/kg). The Electrophoretic Transport interface also adds an equation for the

charge transport in the electrolyte, based on an assumption of electroneutrality, and a set of chemical equilibria describing the water self- ionization reaction and the dissociation reactions of weak acids and bases.

The fluid flow is set up with a Laminar Flow interface, solving for the Navier–Stokes equations.

Results and Discussion

Figure 3 shows the pH in the cell. The pH gradients in the x direction increase toward the outlet.

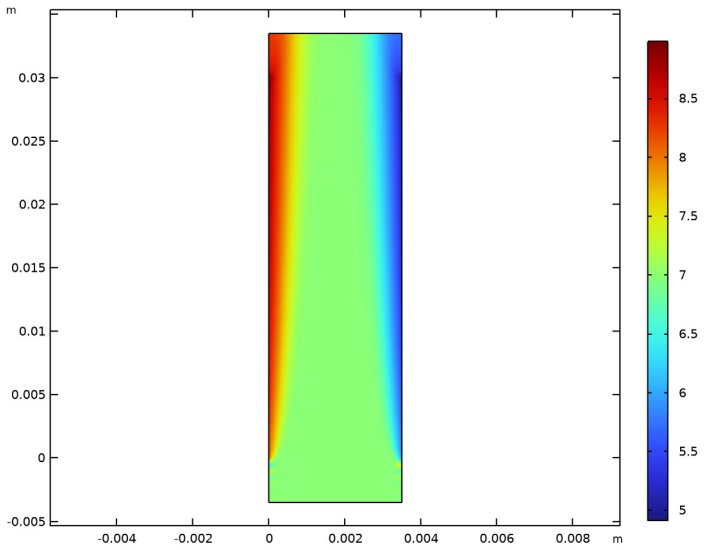


Figure 3: Surface plot of pH in the cell.

Figure 4 shows the electrolyte conductivity. The conductivity gets lower close to the electrode surfaces and toward the outlet due to depletion of charge carriers.

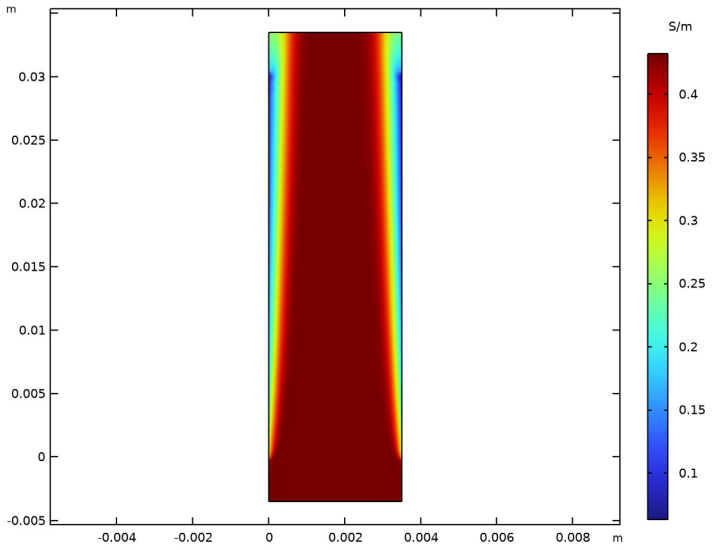


Figure 4: Surface plot of electrolyte conductivity in the cell.

Figure 5 shows the electrolyte potential. Outside the electrode gap, the potential gradients are low, which means that the migrative flux close to the inlet and outlet is low.

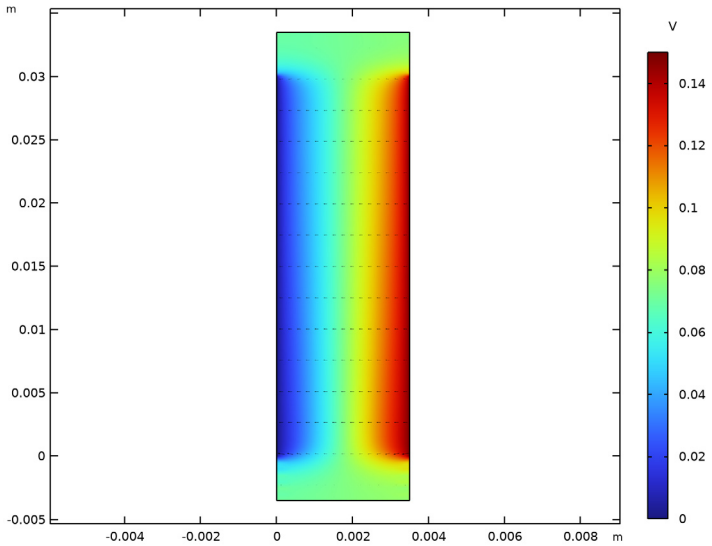


Figure 5: Surface plot of electrolyte potential in the cell.

Figure 6 shows the concentration of Protein 1, which has an isoelectric point of 4.7. The protein is concentrated toward the right electrode.

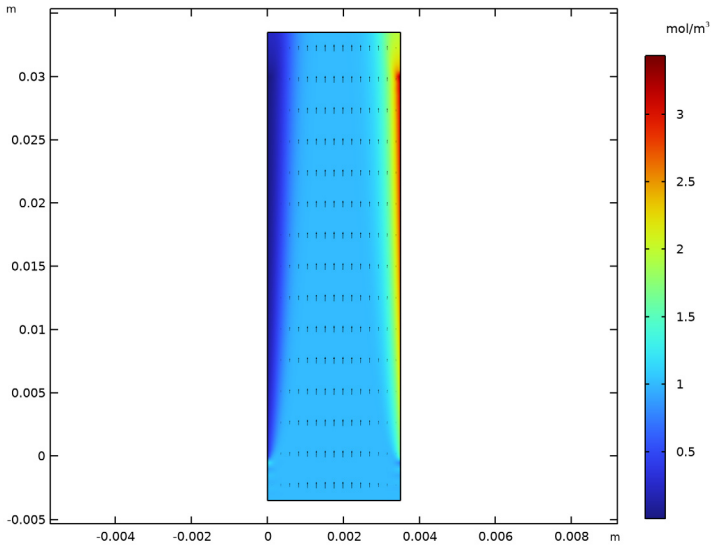


Figure 6: Surface plot of molar concentration of Protein 1 in the cell.

Figure 7 shows the concentration of Protein 2, with an isoelectric point of 6.1. This protein reaches its maximum outlet concentration somewhere between the center and the right electrode.

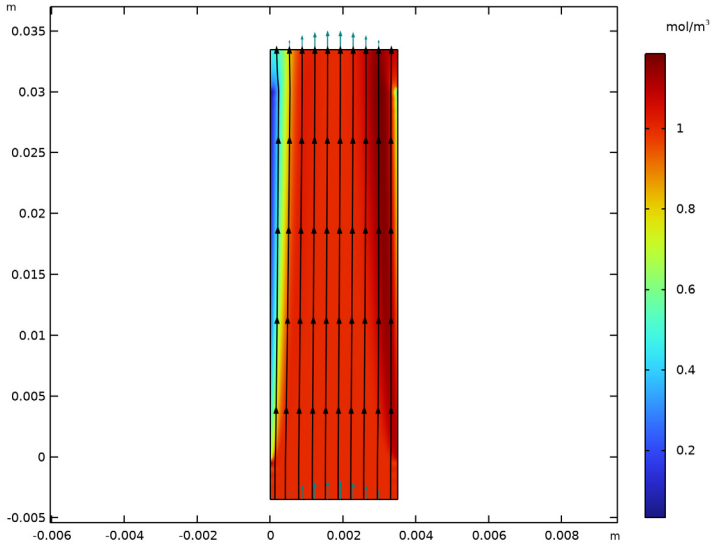


Figure 7: Surface plot of molar concentration of Protein 2 in the cell.

Figure 8 and Figure 9 show the weak acid and base concentrations, respectively. The weak acid, with a negative average charge, is transported to the right and the base, with a positive average charge, is transported to the left in the electric field.

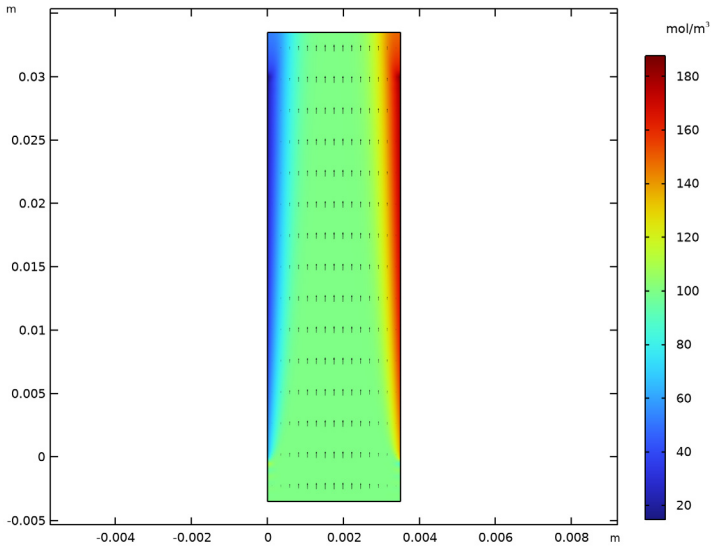


Figure 8: Surface plot of weak acid concentration in the cell.

[

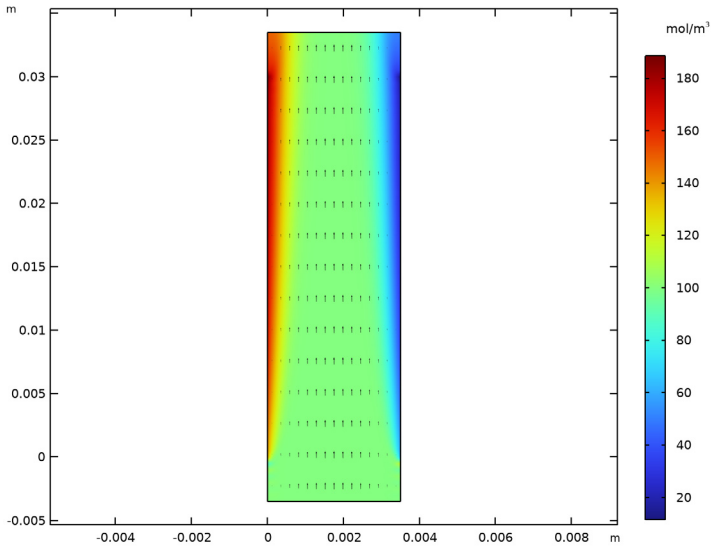


Figure 9: Surface plot of weak base concentration in the cell.

Finally, Figure 10 and Figure 11 show the pH and protein concentration profiles at the outlet.

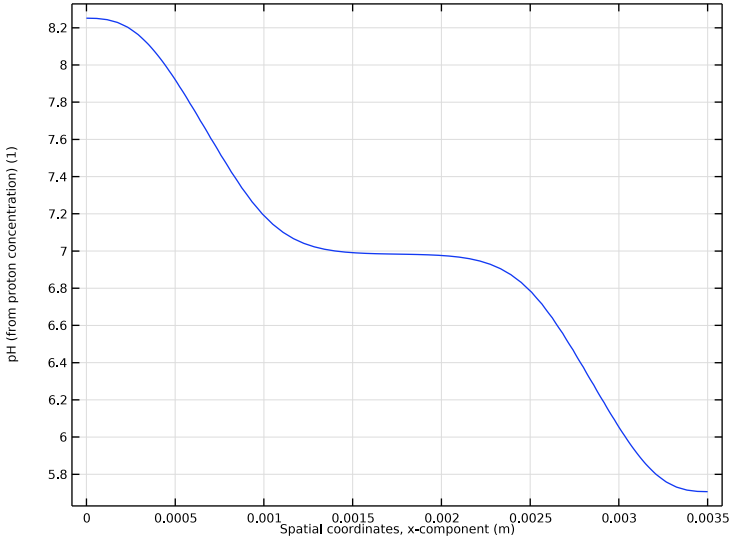


Figure 10: pH profile along the outlet boundary of the cell.

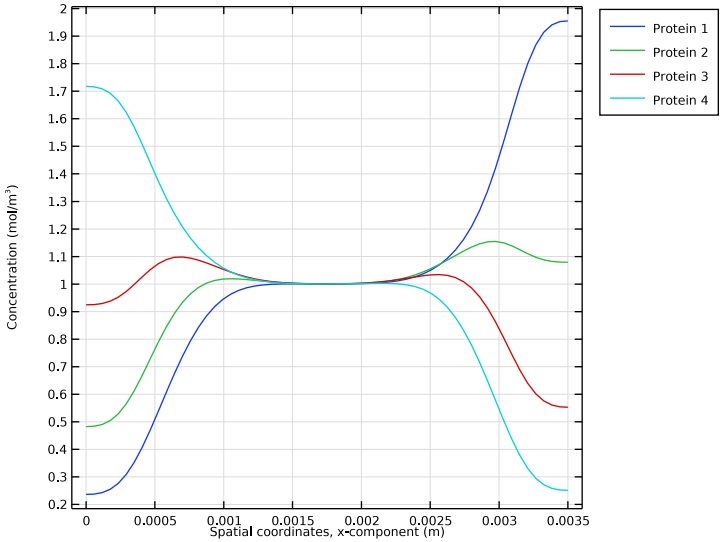


Figure 11: Protein concentration profiles along the outlet boundary of the cell.

Application Library path: `Chemical_Reaction_Engineering_Module/Electrokinetic_Effects/isoelectric_separation`

Modeling Instructions

In this tutorial we couple Electrophoretic Transport to Laminar Flow in 2D. Use the **Model Wizard** to select the space dimension and the physics interfaces. (Studies will be added to the model at a later stage.)

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 **Chemical Species Transport> Electrophoretic Transport (el)**.

3 Click **Add**.

4 In the **Select Physics** tree, select **Fluid Flow>Single-Phase Flow>Laminar Flow (spf)**.

5 Click **Add**.

6 Click **Done**.

GLOBAL DEFINITIONS

Load the model parameters from a text file.

Parameters 1

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 `isoelectric_separation_parameters.txt`.

GEOMETRY 1

Now draw the geometry as a union of three 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 `W`.

4 In the **Height** text field, type `H`.

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`.

4 In the **Height** text field, type `W`.

5 Locate the **Position** section. In the **y** text field, type `-W`.

6 Click **Build Selected**.

7 Right-click **Rectangle 2 (r2)** and choose **Duplicate**.

Rectangle 3 (r3)

1 In the **Model Builder** window, click **Rectangle 3 (r3)**.

2 In the **Settings** window for **Rectangle**, locate the **Position** section.

3 In the **y** text field, type `H`.

4 Click **Build Selected**.

Inlet

Add selections for the inlet and outlet boundaries. These will be used later when setting up the physics.

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

2 In the **Settings** window for **Explicit Selection**, type `Inlet` in the **Label** text field.

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

4 On the object **r2**, select Boundary 1 only.

Outlet

1 In the **Geometry** toolbar, click **Selections** and choose **Explicit Selection**.

2 In the **Settings** window for **Explicit Selection**, type `Outlet` in the **Label** text field.

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

4 On the object **r3**, select Boundary 3 only.

The interior boundaries are not part of the physical geometry. Assign them as **Mesh Control Edges** to make them available in the mesh only.

Mesh Control Edges 1 (mce1)

1 In the **Geometry** toolbar, click **Virtual Operations** and choose **Mesh Control Edges**.

2 On the object **fin**, select Boundaries 4 and 6 only.

3 In the **Settings** window for **Mesh Control Edges**, locate the **Input** section.

4 Clear the **Include adjacent vertices** check box.

5 In the **Geometry** toolbar, click **Build All**.

The model is slender. Change **View scale** to more easily see variations over the entire geometry.

DEFINITIONS

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

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.

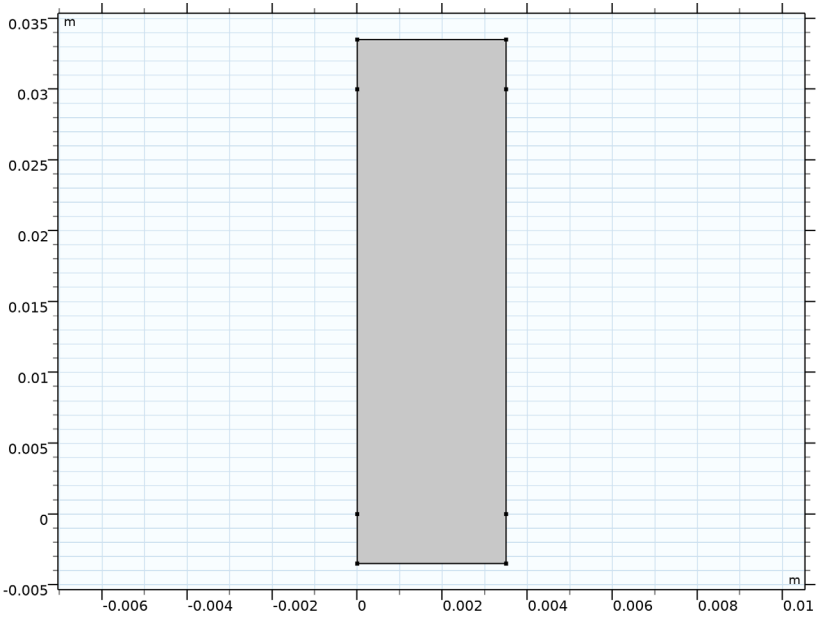
3 From the **View scale** list, choose **Manual**.

4 In the **x scale** text field, type 3.

5 Click **Update**.

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

The finished geometry should now look like this:



MATERIALS

To set up flow equations for the electrolyte we will use some material parameters for water from the **Material Library**.

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 Right-click and choose **Add to Component 1 (comp1)**.

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

ELECTROPHORETIC TRANSPORT (EL)

Now start setting up the **Electrophoretic Transport**.

1 In the **Settings** window for **Electrophoretic Transport**, locate the **Transport Mechanisms** section.

2 Select the **Convection** check box.

Solvent 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Electrophoretic Transport (el)** click **Solvent 1**.

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

3 From the **u** list, choose **Velocity field (spf)**.

Potential 1

This cell is operated potentiostatically (at a constant potential).

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

2 Select Boundary 3 only.

Potential 2

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

2 Select Boundary 7 only.

3 In the **Settings** window for **Potential**, locate the **Electrolyte Potential** section.

4 In the $\phi_{l,bnd}$ text field, type `V0`.

Protein 1

Now add the various species in the electrolyte: 4 proteins, one weak acid and one weak base.

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

2 In the **Settings** window for **Protein**, locate the **Protein** section.

3 In the **Species name** text field, type `p1`.

4 In the **Average charge** text field, type `iep_1-el.pH`.

5 Locate the **Diffusion and Migration** section. In the D text field, type `D_p`.

Inflow 1

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

2 Right-click **Protein 1** and choose **Inflow**.

3 In the **Settings** window for **Inflow**, locate the **Boundary Selection** section.

4 From the **Selection** list, choose **Inlet**.

5 Locate the **Concentration** section. In the c_0 text field, type `cp_in`.

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

Protein 1

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

Outflow 1

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

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

3 From the **Selection** list, choose **Outlet**.

Protein 1

In this tutorial we assume that only the isoelectric point varies between the proteins. Therefore you can just duplicate the first protein to create the second protein, and then and change the average charge.

1 Right-click **Protein 1** and choose **Duplicate**.

Protein 2

1 In the **Model Builder** window, click **Protein 2**.

2 In the **Settings** window for **Protein**, locate the **Protein** section.

3 In the **Species name** text field, type `p2`.

4 In the **Average charge** text field, type `iep_2-el.pH`.

5 Right-click **Protein 2** and choose **Duplicate**.

Protein 3

1 In the **Model Builder** window, click **Protein 3**.

2 In the **Settings** window for **Protein**, locate the **Protein** section.

3 In the **Species name** text field, type `p3`.

4 In the **Average charge** text field, type `iep_3-el.pH`.

5 Right-click **Protein 3** and choose **Duplicate**.

Protein 4

1 In the **Model Builder** window, click **Protein 4**.

2 In the **Settings** window for **Protein**, locate the **Protein** section.

3 In the **Species name** text field, type `p4`.

4 In the **Average charge** text field, type `iep_4-el.pH`.

Weak Acid 1

Finish the electrophoretic transport settings by adding one weak acid and one weak base.

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

2 In the **Settings** window for **Weak Acid**, locate the **Weak Acid** section.

3 In the **Species name** text field, type `wa`.

4 In the pK_a text field, type `pKa_wa`.

5 Locate the **Diffusion and Migration** section. In the u_m text field, type `mob_wa`.

Initial Concentration 1

1 In the **Model Builder** window, expand the **Weak Acid 1** node, then click **Initial Concentration 1**.

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

3 In the c text field, type `cwa_in`.

Weak Acid 1

In the **Model Builder** window, click **Weak Acid 1**.

Inflow 1

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

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

3 From the **Selection** list, choose **Inlet**.

4 Locate the **Concentration** section. In the c_0 text field, type `cwa_in`.

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

Weak Acid 1

In the **Model Builder** window, click **Weak Acid 1**.

Outflow 1

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

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

3 From the **Selection** list, choose **Outlet**.

Weak Base 1

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

2 In the **Settings** window for **Weak Base**, locate the **Weak Base** section.

3 In the **Species name** text field, type `wb`.

4 In the pK_a text field, type `pKa_wb`.

5 Locate the **Diffusion and Migration** section. In the u_m text field, type `mob_wb`.

Initial Concentration 1

1 In the **Model Builder** window, expand the **Weak Base 1** node, then click **Initial Concentration 1**.

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

3 In the c text field, type `cwb_in`.

Weak Base 1

In the **Model Builder** window, click **Weak Base 1**.

Inflow 1

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

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

3 From the **Selection** list, choose **Inlet**.

4 Locate the **Concentration** section. In the c_0 text field, type `cwb_in`.

Weak Base 1

In the **Model Builder** window, click **Weak Base 1**.

Outflow 1

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

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

3 From the **Selection** list, choose **Outlet**.

LAMINAR FLOW (SPF)

Now set up the Laminar Flow interface. Only the boundary conditions need to be specified here since most settings are taken from the Materials node (Water), o.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Laminar Flow (spf)**.

Inlet 1

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

2 Select Boundary 2 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 `Uave`.

Outlet 1

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

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

3 From the **Selection** list, choose **Outlet**.

4 Locate the **Pressure Conditions** section. Select the **Normal flow** check box.

5 Right-click **Outlet 1** and choose **Build All**.

MESH 1

Now set up the mesh. A mapped mesh is suitable since we are using a rectangular geometry.

Mapped 1

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

Distribution 1

1 Right-click **Mapped 1** and choose **Distribution**.

2 Select Boundaries 2, 5, 9, and 10 only.

3 In the **Settings** window for **Distribution**, locate the **Distribution** section.

4 In the **Number of elements** text field, type `60`.

Size

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

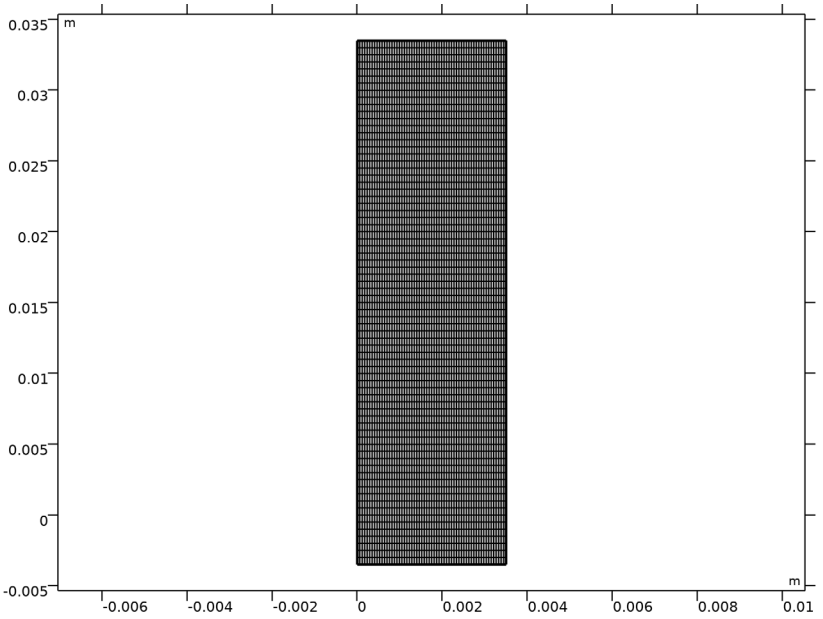
2 In the **Settings** window for **Size**, locate the **Element Size** section.

3 Click the **Custom** button.

4 Locate the **Element Size Parameters** section. In the **Maximum element size** text field, type `5e-4`.

5 Click **Build All**.

The finished mesh should look like this:



ROOT

The model is now ready for solving. In this model the flow is not affected the physics of the **Electrophoretic Transport** interface. Therefore solve the **Laminar Flow** first in a separate study.

ADD STUDY

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

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

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

4 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** check box for **Electrophoretic Transport (el)**.

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

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

STUDY 1 - FLOW CALCULATION

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

2 In the **Settings** window for **Study**, type `Study 1 - Flow Calculation` in the **Label** text field.

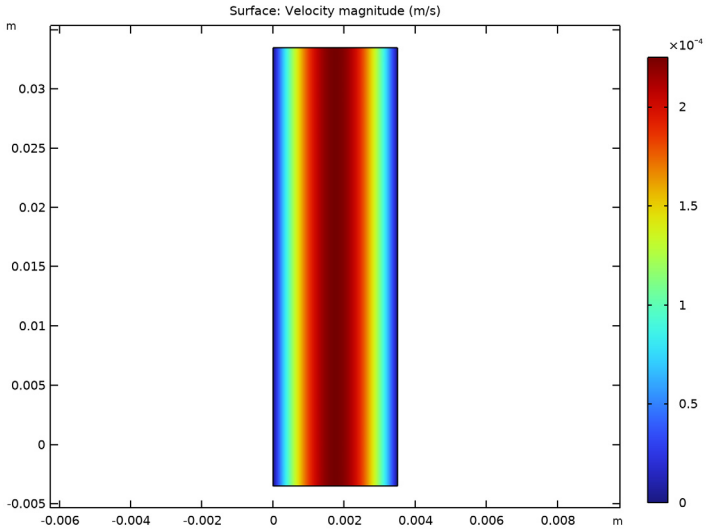
3 In the **Home** toolbar, click **Compute**.

RESULTS

Default plots for the velocity and pressure are generated automatically as follows:

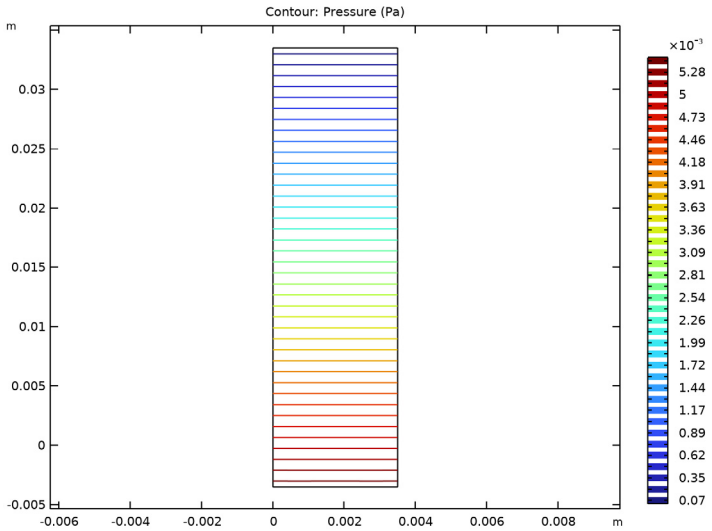
Velocity (spf)

In the **Model Builder** window, under **Results** click **Velocity (spf)**.



Pressure (spf)

In the **Model Builder** window, click **Pressure (spf)**.



ROOT

Add a second study to solve for the **Electrophoretic Transport**, using the solution of the first Study as input for the velocity (and pressure).

ADD STUDY

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

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

3 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** check box for **Laminar Flow (spf)**.

4 Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces>Stationary with Initialization**.

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

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

STUDY 2 - SEPARATION CALCULATION

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

2 In the **Settings** window for **Study**, type `Study 2 - Separation Calculation` in the **Label** text field.

Step 1: Current Distribution Initialization

1 In the **Model Builder** window, under **Study 2 - Separation Calculation** click **Step 1: Current Distribution Initialization**.

2 In the **Settings** window for **Current Distribution Initialization**, click to expand the **Values of Dependent Variables** section.

3 Find the **Values of variables not solved for** subsection. From the **Settings** list, choose **User controlled**.

4 From the **Method** list, choose **Solution**.

5 From the **Study** list, choose **Study 1 - Flow Calculation, Stationary**.

6 In the **Home** toolbar, click = **Compute**.

RESULTS

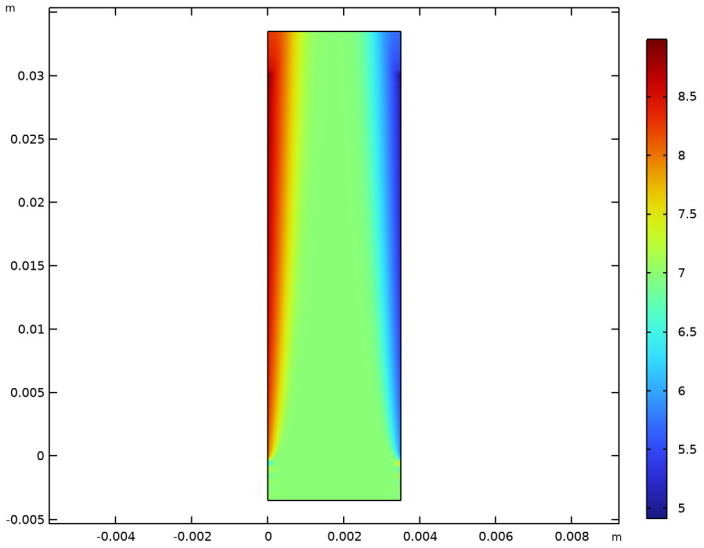
pH (el)

1 In the **Settings** window for **2D Plot Group**, click to expand the **Title** section.

2 From the **Title type** list, choose **None**.

3 Locate the **Color Legend** section. Select the **Show units** check box.

A default pH plot should now have been generated, looking like this:



Electrolyte Conductivity (el)

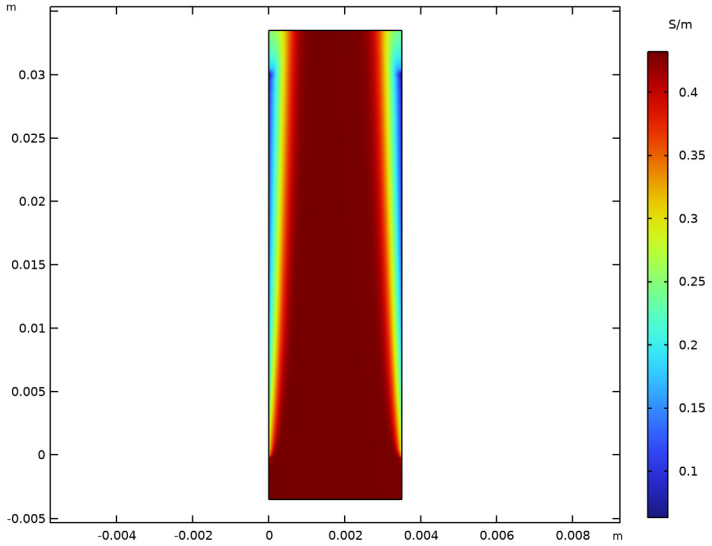
The default electrolyte conductivity plot should look like this:

1 In the **Model Builder** window, click **Electrolyte Conductivity (el)**.

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

3 From the **Title type** list, choose **None**.

4 Locate the **Color Legend** section. Select the **Show units** check box.



Electrolyte Potential (el)

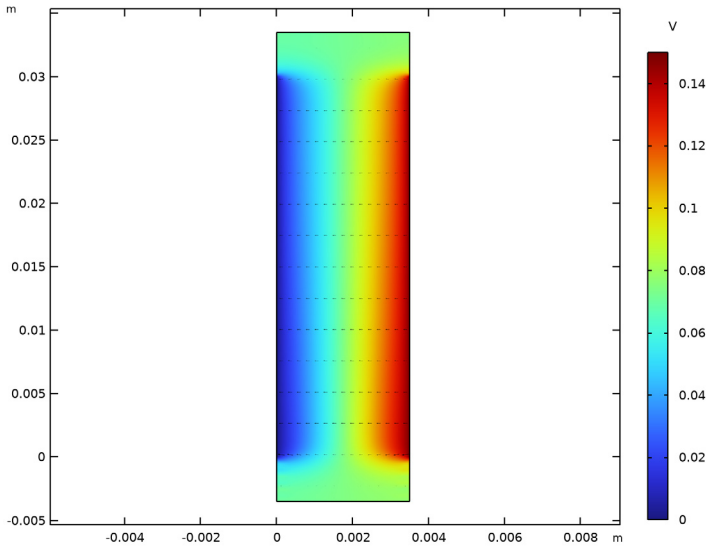
The default electrolyte potential plot should look like this:

1 In the **Model Builder** window, click **Electrolyte Potential (el)**.

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

3 From the **Title type** list, choose **None**.

4 Locate the **Color Legend** section. Select the **Show units** check box.



There should also be six default molar concentration plots present; one for each species in the **Electrophoretic Transport** interface:

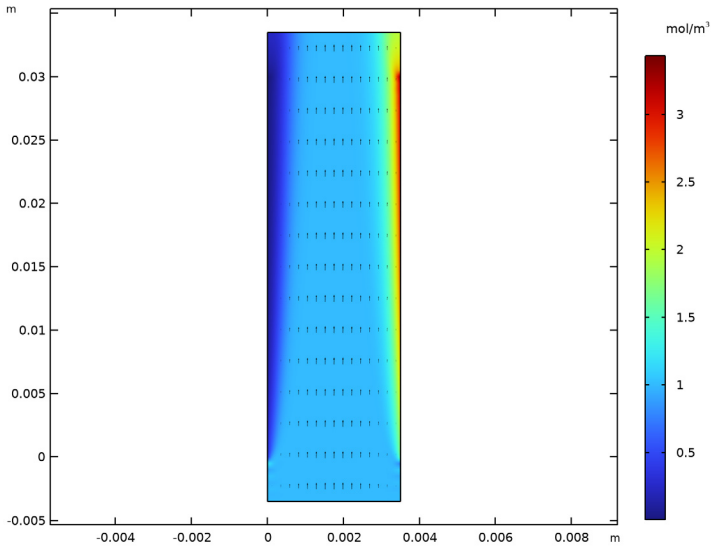
Molar Concentration - p1 (el)

1 In the **Model Builder** window, click **Molar Concentration - p1 (el)**.

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

3 From the **Title type** list, choose **None**.

4 Locate the **Color Legend** section. Select the **Show units** check box.



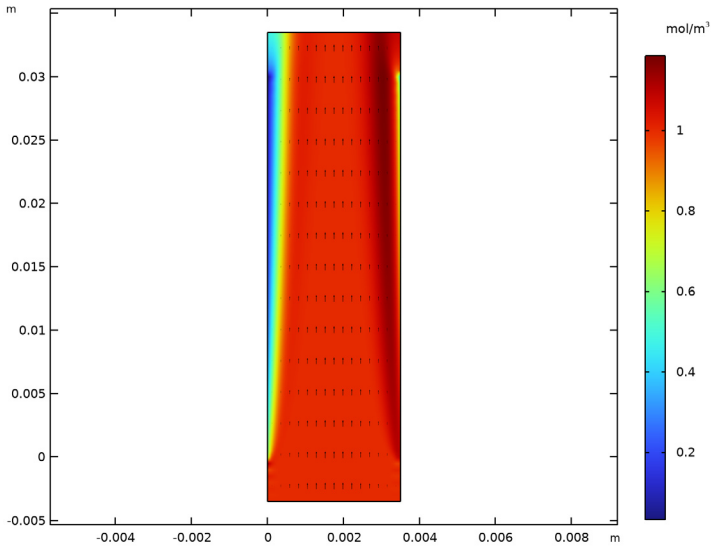
Molar Concentration - p2 (el)

1 In the **Model Builder** window, click **Molar Concentration - p2 (el)**.

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

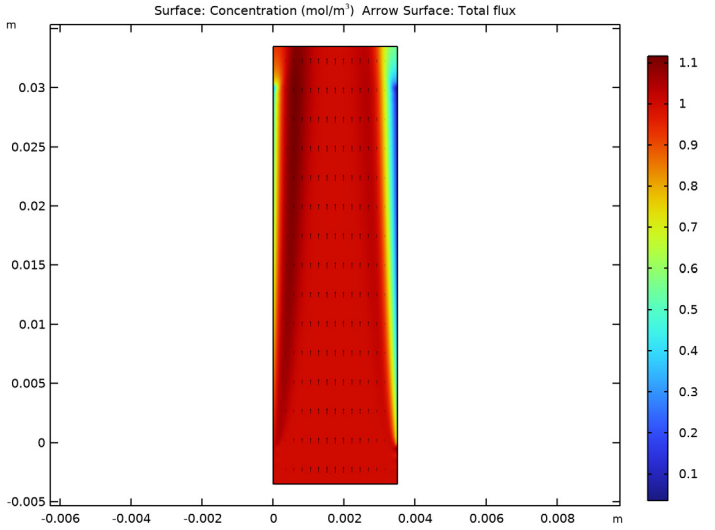
3 From the **Title type** list, choose **None**.

4 Locate the **Color Legend** section. Select the **Show units** check box.



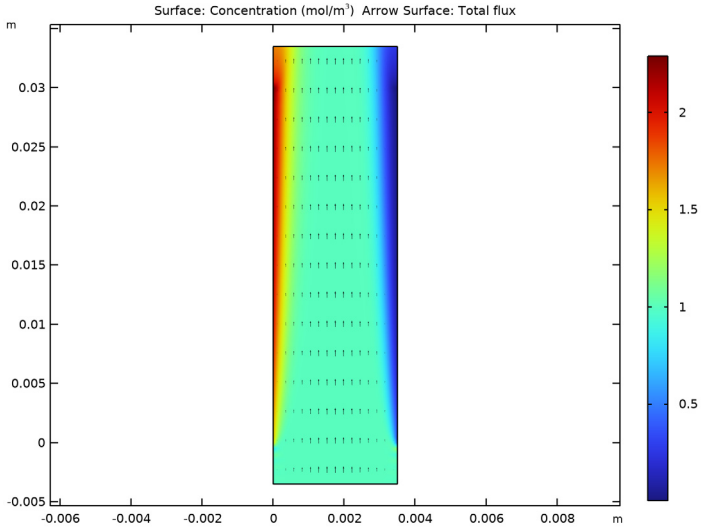
Molar Concentration - p3 (el)

In the **Model Builder** window, click **Molar Concentration - p3 (el)**.



Molar Concentration - p4 (el)

In the **Model Builder** window, click **Molar Concentration - p4 (el)**.



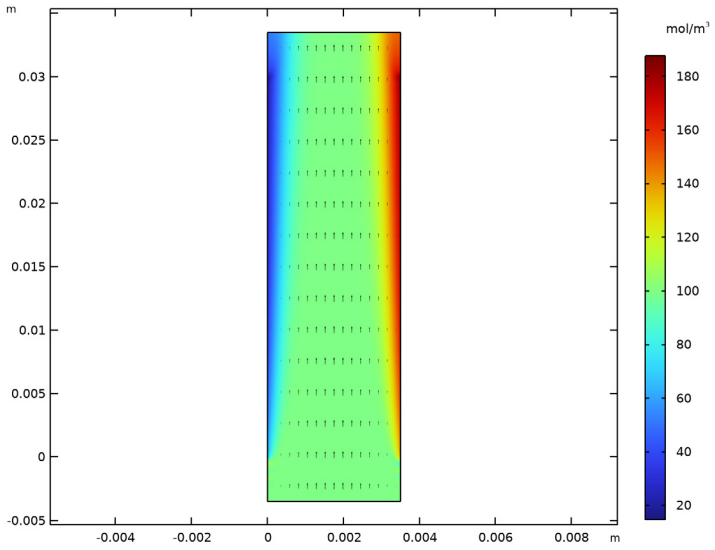
Molar Concentration - wa (el)

1 In the **Model Builder** window, click **Molar Concentration - wa (el)**.

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

3 From the **Title type** list, choose **None**.

4 Locate the **Color Legend** section. Select the **Show units** check box.



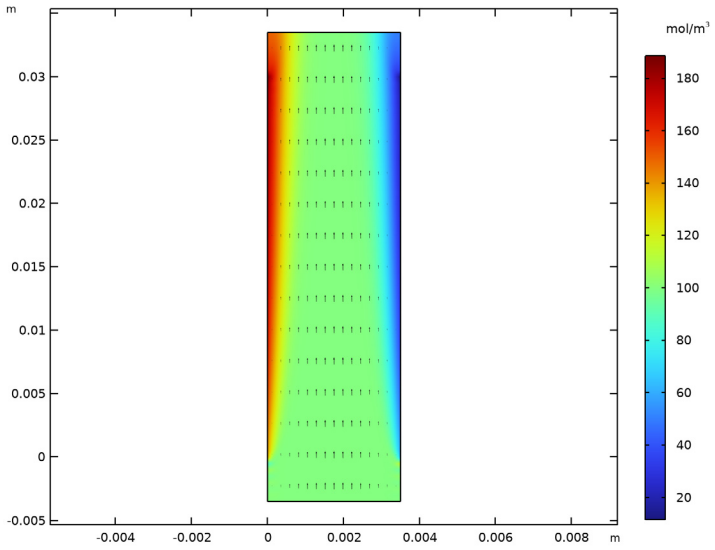
Molar Concentration - wb (el)

1 In the **Model Builder** window, click **Molar Concentration - wb (el)**.

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

3 From the **Title type** list, choose **None**.

4 Locate the **Color Legend** section. Select the **Show units** check box.



Molar Concentration - p2 (el)

Now, to visualize the transport in radial direction, add **Arrow lines** and **Streamlines** to the plot for Protein 2.

Arrow Surface 1

1 In the **Model Builder** window, expand the **Molar Concentration - p2 (el)** node.

2 Right-click **Arrow Surface 1** and choose **Delete**.

Arrow Line 1

1 In the **Model Builder** window, right-click **Molar Concentration - p2 (el)** and choose **Arrow Line**.

2 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)>Laminar Flow> Velocity and pressure>u,v - Velocity field**.

3 Locate the **Arrow Positioning** section. In the **Number of arrows** text field, type 20.

4 Locate the **Coloring and Style** section. From the **Color** list, choose **Custom**.

5 On Windows, click the colored bar underneath, or — if you are running the cross-platform desktop — the **Color** button.

6 Click **Define custom colors**.

7 Set the RGB values to 5, 132, and 133, respectively.

8 Click **Add to custom colors**.

9 Click **Show color palette only** or **OK** on the cross-platform desktop.

10 In the **Molar Concentration - p2 (el)** toolbar, click **Plot**.

Selection 1

1 Right-click **Arrow Line 1** and choose **Selection**.

2 Select Boundaries 2 and 5 only.

3 In the **Molar Concentration - p2 (el)** toolbar, click **Plot**.

Streamline 1

1 In the **Model Builder** window, right-click **Molar Concentration - p2 (el)** and choose **Streamline**.

2 In the **Settings** window for **Streamline**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)> Electrophoretic Transport>Protein 2>el.tflux_p2x,el.tflux_p2y - Total flux**.

3 Locate the **Streamline Positioning** section. In the **Number** text field, type 10.

4 Select Boundary 5 only.

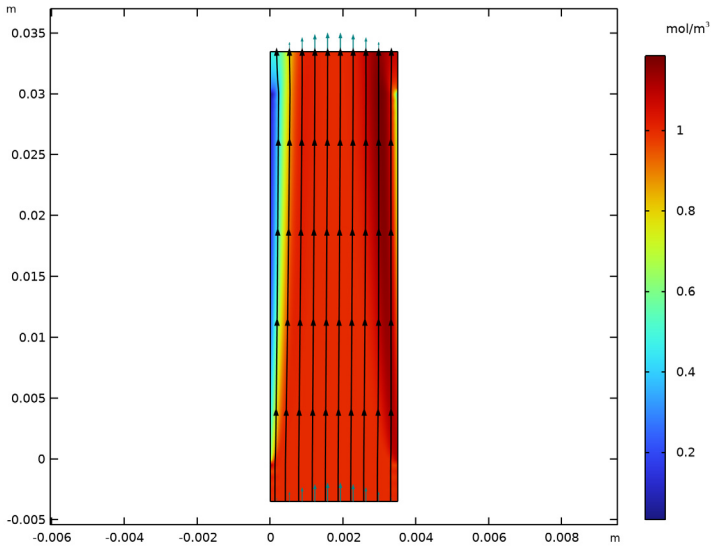
5 Locate the **Coloring and Style** section. Find the **Point style** subsection. From the **Type** list, choose **Arrow**.

6 Select the **Number of arrows** check box. In the associated text field, type 90.

7 Select the **Scale factor** check box. In the associated text field, type 10.

8 In the **Molar Concentration - p2 (el)** toolbar, click **Plot**.

The generated plot should look like this:



pH at Outlet

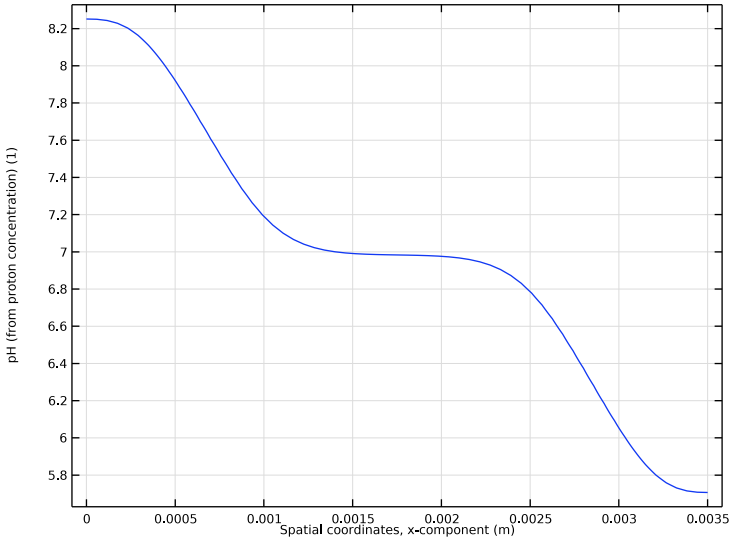
Now proceed to plot the pH at the outlet.

1. In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.
2. In the **Settings** window for **1D Plot Group**, type `pH at Outlet` in the **Label** text field.
3. Locate the **Data** section. From the **Dataset** list, choose **Study 2 - Separation Calculation/ Solution 2 (sol2)**.
4. Click to expand the **Title** section. From the **Title type** list, choose **None**.

Line Graph 1

1. Right-click **pH at Outlet** and choose **Line Graph**.
2. In the **Settings** window for **Line Graph**, locate the **Selection** section.
3. From the **Selection** list, choose **Outlet**.
4. Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.
5. In the **Expression** text field, type `x`.
6. In the **pH at Outlet** toolbar, click **Plot**.

The pH plot should look like this:



Protein Concentrations at Outlet

Finally, create plot of the protein concentrations at the outlet as follows:

1. In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.
2. In the **Settings** window for **1D Plot Group**, type `Protein Concentrations at Outlet` in the **Label** text field.
3. Locate the **Data** section. From the **Dataset** list, choose **Study 2 - Separation Calculation/ Solution 2 (sol2)**.
4. Click to expand the **Title** section. From the **Title type** list, choose **None**.
5. Locate the **Legend** section. From the **Layout** list, choose **Outside graph axis area**.

Line Graph 1

1. Right-click **Protein Concentrations at Outlet** and choose **Line Graph**.
2. In the **Settings** window for **Line Graph**, locate the **Selection** section.
3. From the **Selection** list, choose **Outlet**.
4. Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Electrophoretic Transport>Protein 1>el.c_p1 - Concentration - mol/m³**.
5. Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.
6. In the **Expression** text field, type `x`.

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

8 From the **Legends** list, choose **Manual**.

9 In the table, enter the following settings:

Legends
Protein 1

10 In the **Protein Concentrations at Outlet** toolbar, click **Plot**.

11 Right-click **Line Graph 1** and choose **Duplicate**.

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 `el.c_p2`.

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

Legends
Protein 2

5 Right-click **Line Graph 2** and choose **Duplicate**.

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 `el.c_p3`.

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

Legends
Protein 3

5 Right-click **Line Graph 3** and choose **Duplicate**.

Line Graph 4

1 In the **Model Builder** window, click **Line Graph 4**.

2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type `el.c_p4`.

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

Legends
Protein 4

Protein Concentrations at Outlet

1 In the **Model Builder** window, click **Protein Concentrations at Outlet**.

2 In the **Protein Concentrations at Outlet** toolbar, click **Plot**.

The plot should look like this: