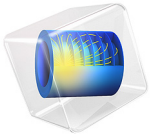

Isoelectric Focusing

Introduction

This model simulates the separation phase during isoelectric focusing of seven carrier ampholytes in a closed column. The pI of the ampholytes uniformly span the interval 3.5–9.5, with ΔpK of 2 for each ampholyte The model reproduces results reported by Thormann and others (Ref. 1).

Model Definition

The model is set up in 1D using the Electrophoretic Transport interface, using seven Ampholyte domain nodes to define the transported species. The same mobility and the same uniform initial concentration values are used for all ampholytes.

The problem is solved in a time-dependent study for the time range 0 to 4 minutes.

Results and Discussion

Figure 1 shows the pH in the column for different times during the simulation. After four minutes the pH profile features seven different plateaus.

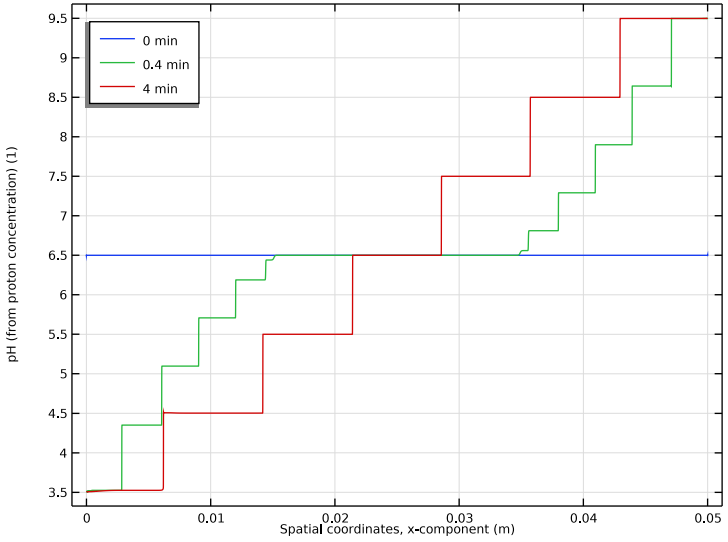

Figure 1: pH of the separation column for various times.

Figure 2 shows the corresponding conductivities in the column. The conductivity decreases as the separation process proceeds.

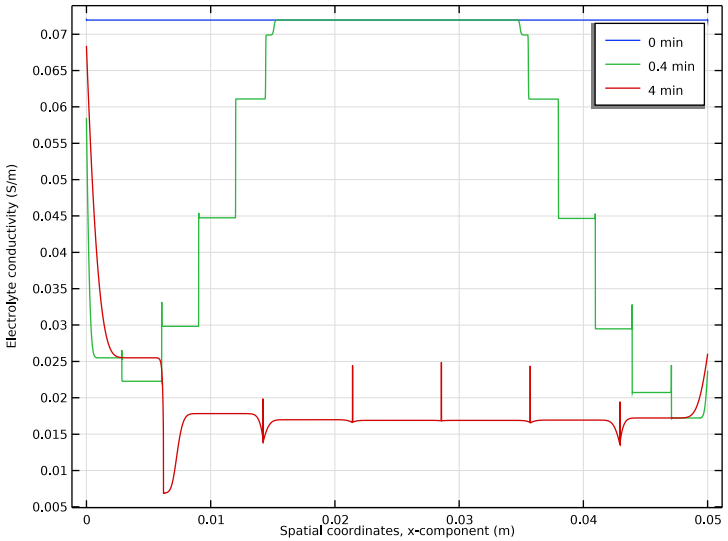

Figure 2: Electrolyte conductivity of the separation column at various times.

Figure 3 shows the current density vs time. The cell is operated at constant voltage conditions, and hence the current density decreases over time as a result of the lowered conductivity.

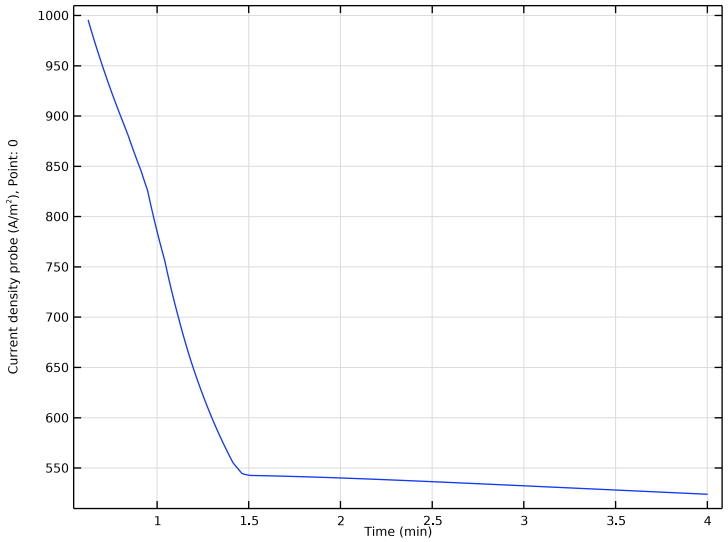

Figure 3: Anode current density (in A/m^2) versus time.

Figure 4 shows the concentration of the seven different ampholytes at $t = 4$ min. At this time, the sample has separated into seven well-separated regions, each one containing one

ampholyte only. Steady-state has however not yet been reached (increase the simulation tome to 3000 s to reach the final concentration profile).

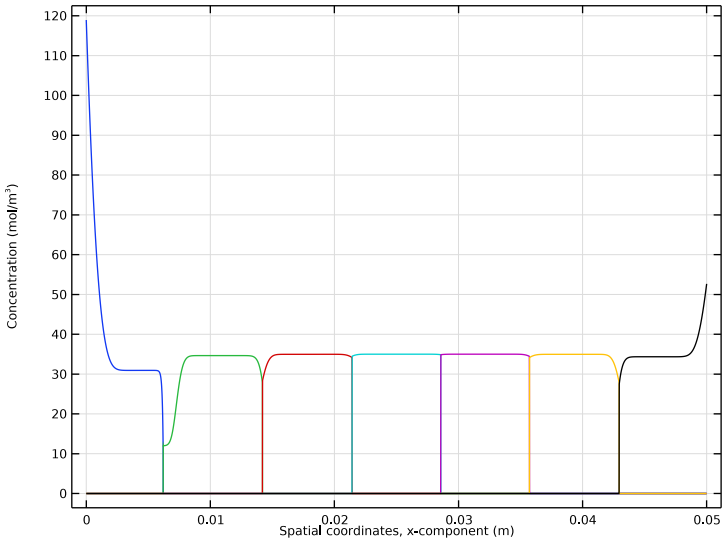

Figure 4: Concentration of the seven ampholytes at t = 4 min.

Reference

1. W. Thormann, M. Breadmore, J. Caslavska, and R. Mosher, "Dynamic computer simulations of electrophoresis: A versatile research and teaching tool," *Electrophoresis*, vol. 31, pp. 726–754, 2010.

Application Library path: `Electrochemistry_Module/Electrochemical_Engineering/isoelectric_focusing_1d`

Modeling Instructions

From the **File** menu, choose **New**.

NEW

In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, click — **1D**.

2 In the **Select Physics** tree, select **Chemical Species Transport> Electrophoretic Transport (el)**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces> Time Dependent with Initialization**.

6 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 `isoelectric_focusing_1d_parameters.txt`.

GEOMETRY 1

Interval 1 (i1)

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Geometry 1** and choose **Interval**.

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

3 In the table, enter the following settings:

Coordinates (m)
0
L

4 Click **Build All Objects**.

ELECTROPHORETIC TRANSPORT (EL)

Potential 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Electrophoretic Transport (el)** and choose **Potential**.

2 Select Boundary 1 only.

Potential 2

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

2 Select Boundary 2 only.

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

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

Ampholyte 1

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

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

3 In the table, enter the following settings:

Dissociation step (1)	pKa (1)
1	`pI_start-1`
2	`pI_start+1`

4 Locate the **Diffusion and Migration** section. In the u_m text field, type `mob`.

Initial Concentration 1

1 In the **Model Builder** window, expand the **Ampholyte 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 `c0`.

Ampholyte 1

In the **Model Builder** window, right-click **Ampholyte 1** and choose **Duplicate**.

Ampholyte 2

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

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

3 In the table, enter the following settings:

Dissociation step (I)	pKa (I)
1	pI_start-1+1
2	pI_start+1+1

4 Right-click **Ampholyte 2** and choose **Duplicate**.

Ampholyte 3

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

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

3 In the table, enter the following settings:

Dissociation step (I)	pKa (I)
1	pI_start-1+2
2	pI_start+1+2

4 Right-click **Ampholyte 3** and choose **Duplicate**.

Ampholyte 4

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

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

3 In the table, enter the following settings:

Dissociation step (I)	pKa (I)
1	pI_start-1+3
2	pI_start+1+3

4 Right-click **Ampholyte 4** and choose **Duplicate**.

Ampholyte 5

1 In the **Model Builder** window, click **Ampholyte 5**.

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

3 In the table, enter the following settings:

Dissociation step (I)	pKa (I)
1	pI_start-1+4
2	pI_start+1+4

4 Right-click **Ampholyte 5** and choose **Duplicate**.

Ampholyte 6

1 In the **Model Builder** window, click **Ampholyte 6**.

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

3 In the table, enter the following settings:

Dissociation step (1)	pKa (1)
1	pI_start-1+5
2	pI_start+1+5

4 Right-click **Ampholyte 6** and choose **Duplicate**.

Ampholyte 7

1 In the **Model Builder** window, click **Ampholyte 7**.

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

3 In the table, enter the following settings:

Dissociation step (1)	pKa (1)
1	pI_start-1+6
2	pI_start+1+6

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

Proceed as follows to create a user-defined mesh with a higher resolution toward the end boundaries:

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

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

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

Size

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

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

3 Click the **Custom** button.

4 Locate the **Element Size Parameters** section. In the **Maximum element size** text field, type `4e-6`.

Size 1

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

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

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

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

5 Locate the **Element Size** section. Click the **Custom** button.

6 Locate the **Element Size Parameters** section.

7 Select the **Maximum element size** check box. In the associated text field, type `1e-6`.

8 Click **Build All**.

The model is now ready for solving. Add a probe to monitor the current density for each time step during the simulation.

DEFINITIONS

Domain Point Probe 1

1 In the **Definitions** toolbar, click **Probes** and choose **Domain Point Probe**.

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

3 Select the **Snap to closest point** check box.

Point Probe Expression 1 (ppb1)

1 In the **Model Builder** window, expand the **Domain Point Probe 1** node, then click **Point Probe Expression 1 (ppb1)**.

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

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

4 Select the **Description** check box. In the associated text field, type `Current density probe`.

STUDY 1

Step 2: Time Dependent

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

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

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

4 In the **Output times** text field, type `0 0.4 4`.

The initial transients of the focusing process will be very short. Modify the default solver to set a small initial time step.

Solution 1 (sol1)

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

2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node, then click **Time-Dependent Solver 1**.

3 In the **Settings** window for **Time-Dependent Solver**, click to expand the **Time Stepping** section.

4 Select the **Initial step** check box. In the associated text field, type `1e-5`.

The model will take a few hours to solve.

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

RESULTS

pH (el)

A number of default plots are created by default.

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

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

3 Locate the **Legend** section. From the **Position** list, choose **Upper left**.

Electrolyte Conductivity (el)

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

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

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

Current Density vs. Time

1 In the **Model Builder** window, under **Results** click **Probe Plot Group 1**.

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

3 Locate the **Legend** section. Clear the **Show legends** check box.

Molar Concentration - S (el)

Proceed as follows to create a plot of all ampholyte concentrations in the same figure:

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

Concentrations

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

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

3 Locate the **Data** section. From the **Time selection** list, choose **Last**.

4 Click to expand the **Title** section. From the **Title type** list, choose **None**.

Line Graph 1

1 In the **Model Builder** window, expand the **Concentrations** node, then click **Line Graph 1**.

2 In the **Settings** window for **Line Graph**, click to expand the **Legends** section.

3 Clear the **Show legends** check box.

4 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_S1`.

4 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_S2`.

4 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_S3`.

4 Right-click **Line Graph 4** and choose **Duplicate**.

Line Graph 5

1 In the **Model Builder** window, click **Line Graph 5**.

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

3 In the **Expression** text field, type `el.c_S4`.

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

Line Graph 6

1 In the **Model Builder** window, click **Line Graph 6**.

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

3 In the **Expression** text field, type `el.c_S5`.

4 Right-click **Line Graph 6** and choose **Duplicate**.

Line Graph 7

1 In the **Model Builder** window, click **Line Graph 7**.

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

3 In the **Expression** text field, type `el.c_S6`.

4 In the **Concentrations** toolbar, click  **Plot**.