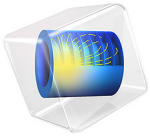

Separation Through Dialysis

Introduction

Dialysis is a widely used separation method. An example is hemodialysis, where membranes are used as artificial kidneys for people with renal failure. Other applications include the recovery of caustic colloidal hemicellulose during viscose manufacturing as well as the removal of alcohol from beer (Ref. 1).

In the dialysis process specific components are preferentially transported through a membrane. The process is diffusion-driven, that is, components diffuse through a membrane due to concentration differences between the dialysate and the permeate sides of the membrane. Separation between solutes is achieved as a result of the different diffusion rates across the membrane, which arise from differences in molecular size and solubility.

This example examines a process aimed at lowering the concentration of a contaminant component in an aqueous product stream. The dialysis equipment is made of a hollow fiber module, where a large number of hollow fibers act as the membrane. It focuses on the transport of the contaminant in the hollow fiber and through its wall.

Figure 1 shows a diagram of the hollow fiber assembly within a dialysis module where the dialysate flows inside while the permeate flows on the outside in a co-current manner. The contaminant is transported through the fiber walls to the permeate side. Species with a higher molecular weight are retained in the dialysate side, due to their low solubility and diffusivity through the membrane.

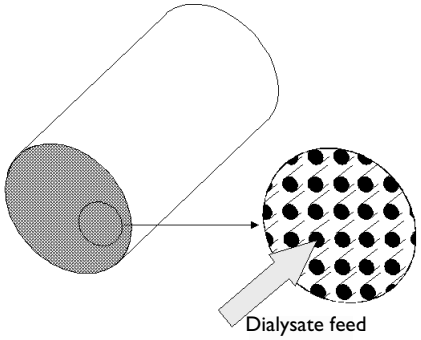

Figure 1: The hollow fiber assembly in a dialysis module.

Model Definition

This example models a piece of hollow fiber through which the dialysate flows with a fully developed laminar parabolic velocity profile. The fiber is surrounded by a permeate that flows laminarly in the same direction as the dialysate.The dialysate, the permeate, and the membrane are all examined in the results. The model domain is shown in Figure 2.Here, the angular gradients are considered negligible, so an axisymmetrical approximation can be used.

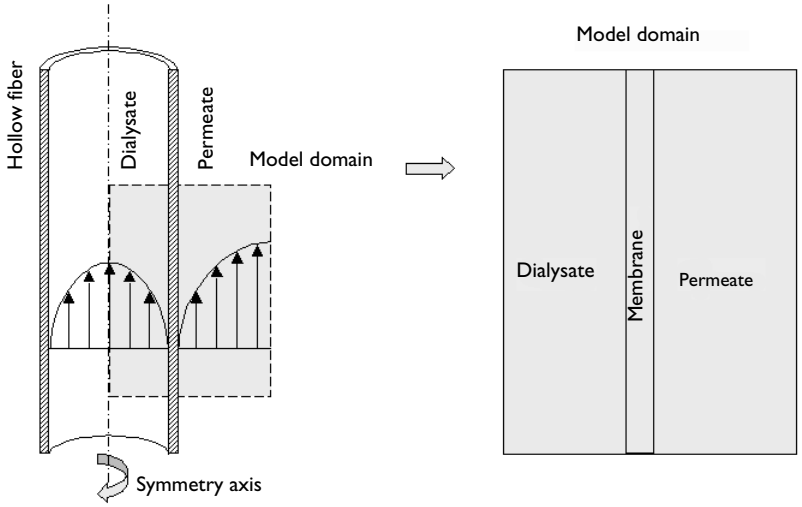

Figure 2: Illustrations of the hollow fiber setup with the dialysate and permeate, and of the model domain.

You can draw a hexagonal-shaped unit cell of the fiber assembly as in Figure 3:

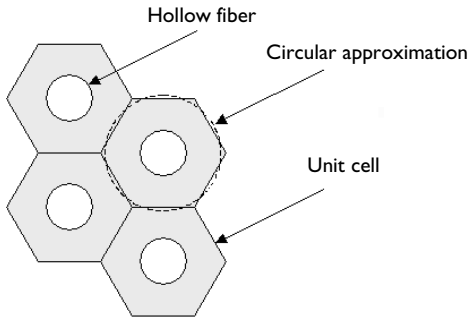

Figure 3: Hexagonal-shaped unit cell of the fiber assembly.

As a simplification, the hexagon is approximated as a circle in the model.

The contaminant is transported by diffusion and convection within the two liquids, whereas diffusion is the only transport mechanism through the membrane. The mass transport is modeled with the Transport of Diluted Species interface. To analyze the convective flux, the Laminar Flow interface is utilized, assuming that the flow is laminar.

The contaminant must dissolve into the membrane in order to be transported through it. The interface conditions between the liquids and the membrane are described by the dimensionless partition coefficient K:

$$K = \frac{c_2^{\mathrm{d}}}{c_1^{\mathrm{d}}} = \frac{c_3^{\mathrm{p}}}{c_4^{\mathrm{p}}} \tag{1}$$

where c_i denotes the concentration of the contaminant (SI unit: $\mathrm{mol/m^3}$). The subscripts and superscripts describe the location in the dialysis fiber as displayed in Figure 4. This figure also shows a schematic concentration profile.

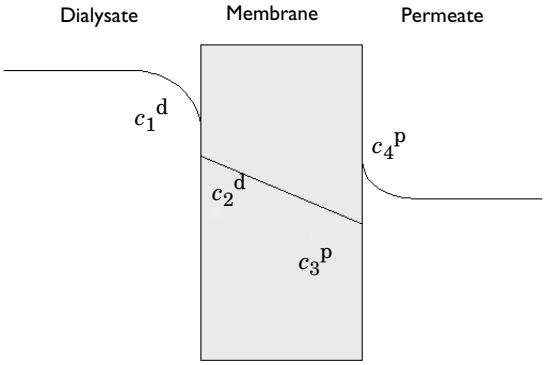

Figure 4: The concentration profile across the membrane (see Equation 1). Note that there are discontinuities in the concentration profile at the membrane boundaries.

To obtain a well-posed problem, an appropriate set of boundary conditions must be defined. Figure 5 displays the boundaries that need to be accounted for. Note that the concentration is discontinuous at the membrane-liquid interfaces; boundary conditions need to be set on both sides of the interface. Equation 1 is implemented at each of the two boundaries using a Partition Condition node. In addition to prescribing the concentration ratio, this node ensures that the mass flux is identical on both sides of the interface.

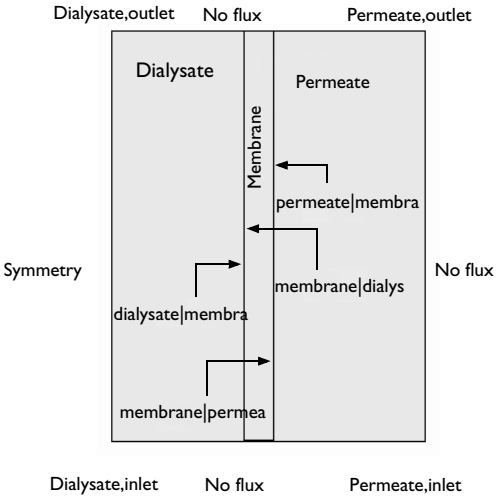

Figure 5: The boundaries accounted for in the model.

Danckwerts' inflow conditions are set at the inlet to the dialysate and permeate. At the outlet, the convective contribution to the mass transport is assumed to be much larger than the diffusive contribution and is modeled by setting outflow conditions. Symmetry applies at the leftmost boundary for this axisymmetrical model geometry and no flux is set at the membrane edges and the rightmost boundary, since no species pass these.

SUMMARY OF INPUT DATA

The input data are listed in the table:

PROPERTY	VALUE	DESCRIPTION
D	10^{-9} m^2/s	Diffusion coefficient, liquids
D_m	10^{-9} m^2/s	Diffusion coefficient, membrane
R_{hf}	0.2 mm	Inner radius, hollow fiber
L_m	0.28 mm	Thickness, membrane
L_{pc}	0.7 mm	Width, concentric permeate channel
H	21 mm	Length, fiber
U_{ave_dia}	0.5 mm/s	Average velocity, dialysate
U_{ave_per}	0.8 mm/s	Average velocity, permeate
K	0.7	Partition coefficient
c_0	1 M	Inlet concentration, dialysate

Results and Discussion

The surface plot in Figure 6 visualizes the concentration distribution throughout the three model domains in 3D: the dialysate liquid inside the hollow fiber (nearest the center), the membrane, and the permeate liquid outside the hollow fiber. As the plot shows, the concentration inside the hollow fiber decreases markedly over the first 10 mm from the inlet. The contaminant transport, starting from the dialysate inlet, is shown in detail in Figure 7. In this figure the radial direction has been rescaled for clarity. Streamlines of the total flux of the contaminant is plotted, with arrows separated by a fixed time interval. Observing the number of arrows inside the membrane, it is evident that the time for the transport across the membrane increases with the downstream distance. This occurs since the driving force, the concentration difference between the dialysate and the permeate side, decreases with the downstream direction.

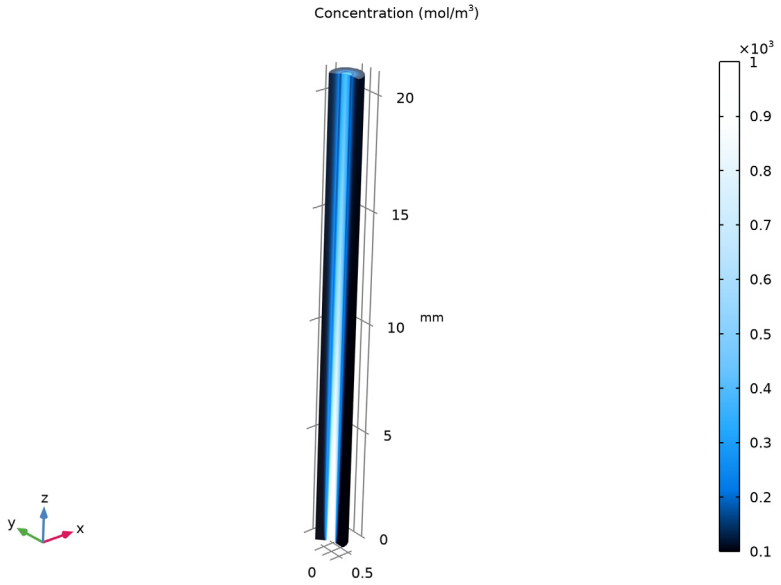

Figure 6: Concentration in the three domains using a revolution dataset.

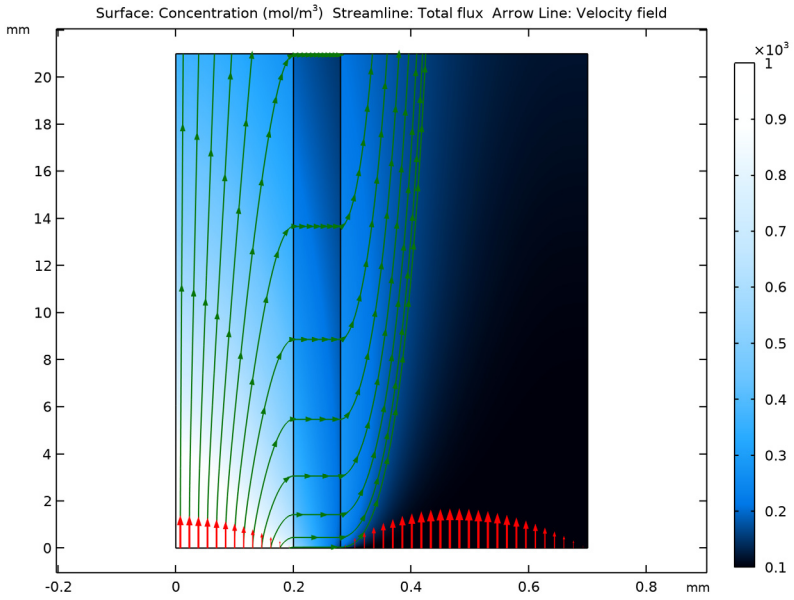

Figure 7: Contaminant development using a scaled radial direction. The streamlines show the total flux with arrows positioned using a fixed time interval.

Concentration jumps arise at the boundaries between the domains. This is shown in Figure 8 where the concentration profile at the middle of the fiber length is plotted along the radius of the model geometry.

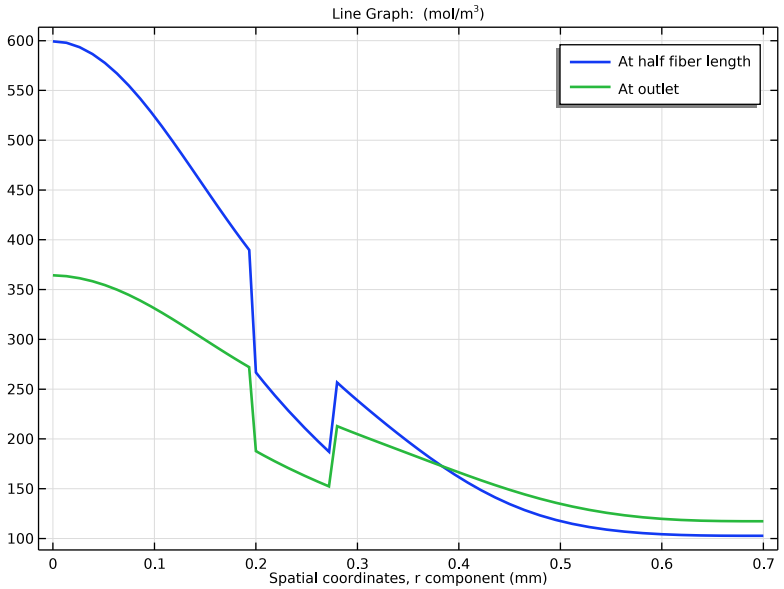

Figure 8: Concentration across the three domains at the middle of the fiber length and at the outlet.

References

1. M. Mulder, *Basic Principles of Membrane Technology*, 2nd ed., Kluwer Academic Publishers, 1998.

2. R.B. Bird, W.E. Stewart, and E.N. Lightfoot, *Transport Phenomena*, John Wiley & Sons, 1960.

Application Library path: `Chemical_Reaction_Engineering_Module/Mixing_and_Separation/dialysis`

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

NEW

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

MODEL WIZARD

1 In the **Model Wizard** window, click **2D Axisymmetric**.

2 In the **Select Physics** tree, select **Chemical Species Transport> Transport of Diluted Species (tds)**.

3 Click **Add**.

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

5 Click **Add**.

6 Click **Study**.

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

8 Click **Done**.

ROOT

Load parameters from a text-file.

GLOBAL DEFINITIONS

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 `dialysis_parameters.txt`.

Draw the geometry and make selections.

GEOMETRY 1

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

2 In the **Settings** window for **Geometry**, locate the **Units** section.

3 From the **Length unit** list, choose **mm**.

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 `Rhf`.

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

5 Click **Build Selected**.

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

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 `Lm`.

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

5 Locate the **Position** section. In the **r** text field, type `Rhf`.

6 Click **Build Selected**.

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

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 `Lpc`.

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

5 Locate the **Position** section. In the **r** text field, type `Rhf+Lm`.

6 Click **Build Selected**.

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

Form Union (fin)

1 In the **Model Builder** window, click **Form Union (fin)**.

2 In the **Settings** window for **Form Union/Assembly**, click **Build Selected**.

Dialysate and Permeate

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

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

3 On the object **fin**, select Domains 1 and 3 only.

Membrane

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

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

3 On the object **fin**, select Domain 2 only.

Model transport by convection and diffusion in the dialysate and permeate, and diffusion in the membrane.

TRANSPORT OF DILUTED SPECIES (TDS)

Transport Properties - Dialysate and Permeate

1 In the **Model Builder** window, under **Component 1 (comp1)>** **Transport of Diluted Species (tds)** click **Transport Properties 1**.

2 In the **Settings** window for **Transport Properties**, type `Transport Properties - Dialysate and Permeate` in the **Label** text field.

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

4 Locate the **Diffusion** section. In the D_c text field, type `D`.

Transport Properties - Membrane

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

2 Select Domain 2 only.

3 In the **Settings** window for **Transport Properties**, type `Transport Properties - Membrane` in the **Label** text field.

4 Locate the **Diffusion** section. In the D_c text field, type `Dm`.

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 *c* text field, type `c0_dia`.

Initial Values 2

1 Right-click **Component 1 (comp1)>Transport of Diluted Species (tds)>Initial Values 1** and choose **Duplicate**.

2 Select Domain 3 only.

3 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

4 In the *c* text field, type `c0_per`.

Inflow 1

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

2 Select Boundary 2 only.

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

4 In the $c_{0,c}$ text field, type `c0_dia`.

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

Inflow 2

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

2 Select Boundary 8 only.

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

4 In the $c_{0,c}$ text field, type `c0_per`.

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 Select Boundaries 3 and 9 only.

Add a **Partition Condition** feature to implement the concentration ratio at the dialysate-membrane interface.

Partition Condition 1

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

2 Select Boundary 4 only.

3 In the **Settings** window for **Partition Condition**, locate the **Partition Condition** section.

4 In the K_c text field, type `K`.

Note that up and downside for the concentration are indicated in the **Graphics window**. The arrow, situated on the selected boundary, points from the downside into the upside. In this case let the membrane side correspond to the upside to achieve the desired condition.

Add another **Partition Condition** feature to implement the concentration ratio at the permeate-membrane interface.

Partition Condition 2

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

2 Select Boundary 7 only.

Use the **Reverse direction** check box to make the membrane side correspond to the upside also for this condition.

3 In the **Settings** window for **Partition Condition**, locate the **Partition Condition** section.

4 Find the **Boundary normal** subsection. Select the **Reverse direction** check box.

5 In the K_c text field, type K.

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 **Liquids and Gases>Liquids>Water**.

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

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

LAMINAR FLOW (SPF)

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

2 In the **Settings** window for **Laminar Flow**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Dialysate and Permeate**.

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_dia`.

Inlet 2

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

2 Select Boundary 8 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_per`.

Outlet 1

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

2 Select Boundaries 3 and 9 only.

3 In the **Settings** window for **Outlet**, locate the **Pressure Conditions** section.

4 Select the **Normal flow** check box.

MESH 1

Mapped 1

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

Distribution 1

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

2 Select Boundaries 1, 4, 7, and 10 only.

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

4 From the **Distribution type** list, choose **Predefined**.

5 In the **Number of elements** text field, type 250.

6 In the **Element ratio** text field, type 25.

Distribution 2

1 In the **Model Builder** window, right-click **Mapped 1** and choose **Distribution**.

2 Select Boundaries 5 and 6 only.

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

4 From the **Distribution type** list, choose **Predefined**.

5 In the **Number of elements** text field, type 7.

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

7 Select the **Symmetric distribution** check box.

Distribution 3

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

2 Select Boundaries 2 and 3 only.

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

4 From the **Distribution type** list, choose **Predefined**.

5 In the **Number of elements** text field, type 20.

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

Distribution 4

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

2 Select Boundary 9 only.

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

4 Select Boundaries 8 and 9 only.

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

6 From the **Distribution type** list, choose **Predefined**.

7 In the **Number of elements** text field, type 30.

8 In the **Element ratio** text field, type 3.

9 Select the **Reverse direction** check box.

Solve the model in two steps. First, the **Laminar Flow** interface and thereafter the **Transport of Diluted Species** interface.

STUDY 1

Step 1: Stationary

1 In the **Model Builder** window, under **Study 1** click **Step 1: Stationary**.

2 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.

3 In the table, clear the **Solve for** check box for **Transport of Diluted Species (tds)**.

Stationary 2

1 In the **Study** toolbar, click **Study Steps** and choose **Stationary>Stationary**.

2 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.

3 In the table, clear the **Solve for** check box for **Laminar Flow (spf)**.

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

RESULTS

Concentration (tds)

1 Click the **Show More Options** button in the **Model Builder** toolbar.

2 In the **Show More Options** dialog box, in the tree, select the check box for the node **Results>Views**.

3 Click **OK**.

View 2D 2

In the **Model Builder** window, under **Results** right-click **Views** and choose **View 2D**.

Axis

1 In the **Model Builder** window, expand the **View 2D 2** 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 25.

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

Concentration (tds)

1 In the **Model Builder** window, under **Results** click **Concentration (tds)**.

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

3 From the **View** list, choose **View 2D 2**.

4 In the **Concentration (tds)** toolbar, click  **Plot**.

Surface 1

1 In the **Model Builder** window, expand the **Concentration (tds)** node, then click **Surface 1**.

2 In the **Settings** window for **Surface**, locate the **Coloring and Style** section.

3 From the **Color table** list, choose **JupiterAuroraBorealis**.

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

Streamline 1

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

2 In the **Settings** window for **Streamline**, locate the **Streamline Positioning** section.

3 From the **Positioning** list, choose **On selected boundaries**.

4 In the **Number** text field, type 13.

5 Locate the **Selection** section. Click to select the **Activate Selection** toggle button.

6 Select Boundary 2 only.

7 Locate the **Coloring and Style** section. Find the **Point style** subsection. From the **Arrow distribution** list, choose **Equal time**.

8 From the **Arrow length** list, choose **Normalized**.

9 Select the **Scale factor** check box.

10 In the associated text field, type 2.

11 From the **Color** list, choose **Custom**.

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

13 Click **Define custom colors**.

14 Set the RGB values to 9, 118, and 9, respectively.

15 Click **Add to custom colors**.

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

Arrow Line 1

In the **Model Builder** window, right-click **Concentration (tds)** and choose **Arrow Line**.

Selection 1

1 In the **Model Builder** window, right-click **Arrow Line 1** and choose **Selection**.

2 Select Boundaries 2 and 8 only.

Arrow Line 1

1 In the **Model Builder** window, click **Arrow Line 1**.

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,w - Velocity field**.

3 Locate the **Arrow Positioning** section. In the **Number of arrows** text field, type 39.

4 Locate the **Coloring and Style** section. Select the **Scale factor** check box.

5 In the associated text field, type 1400.

6 In the **Concentration (tds)** toolbar, click **Plot**.

Concentration 2D Revolution

1 In the **Model Builder** window, under **Results** click **Concentration, 3D (tds)**.

2 In the **Settings** window for **3D Plot Group**, type `Concentration 2D Revolution` in the **Label** text field.

3 Locate the **Plot Settings** section. Clear the **Plot dataset edges** check box.

Surface 1

1 In the **Model Builder** window, expand the **Concentration 2D Revolution** node, then click **Surface 1**.

2 In the **Settings** window for **Surface**, locate the **Coloring and Style** section.

3 From the **Color table** list, choose **JupiterAuroraBorealis**.

If necessary, the view angle of the plot can be adjusted with the mouse.

Concentration 2D Revolution

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

2 In the **Model Builder** window, click **Concentration 2D Revolution**.

3 In the **Concentration 2D Revolution** toolbar, click **Plot**.

Surface

1 In the **Model Builder** window, expand the **Velocity (spf)** node, then click **Surface**.

2 In the **Settings** window for **Surface**, locate the **Coloring and Style** section.

3 From the **Color table** list, choose **Wave**.

Visualize the pressure contours in the dialysate and permeate separately.

Selection 1

1 In the **Model Builder** window, expand the **Pressure (spf)** node.

2 Right-click **Contour** and choose **Selection**.

3 Select Domain 3 only.

Contour

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

2 In the **Settings** window for **Contour**, locate the **Levels** section.

3 In the **Total levels** text field, type 20.

Contour 2

Right-click **Contour** and choose **Duplicate**.

Selection 1

1 In the **Model Builder** window, expand the **Contour 2** node, then click **Selection 1**.

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

3 Click  **Clear Selection**.

4 Select Domain 1 only.

5 In the **Pressure (spf)** toolbar, click  **Plot**.

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

Velocity 2D Revolution

1 In the **Model Builder** window, under **Results** click **Velocity, 3D (spf)**.

2 In the **Settings** window for **3D Plot Group**, type `Velocity 2D Revolution` in the **Label** text field.

Surface

1 In the **Model Builder** window, expand the **Velocity 2D Revolution** node, then click **Surface**.

2 In the **Settings** window for **Surface**, locate the **Coloring and Style** section.

3 From the **Color table** list, choose **Wave**.

Create cut lines at two locations along the fiber length to illustrate the concentration jump between the domains in Figure 8.

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 **z** to `H/2`.

4 In row **Point 2**, set **r** to `Rhf+Lm+Lpc` and **z** to `H/2`.

Cut Line 2D 2

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 **z** to `H`.

4 In row **Point 2**, set **r** to `Rhf+Lm+Lpc` and **z** to `H`.

Concentration Jump

1 In the **Results** toolbar, click **1D Plot Group**.

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

At H/2

1 Right-click **Concentration Jump** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, type `At H/2` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Cut Line 2D 1**.

4 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

5 In the **Expression** text field, type `r`.

6 Click to expand the **Coloring and Style** section. In the **Width** text field, type `2`.

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
`At half fiber length`

At H

1 In the **Model Builder** window, right-click **Concentration Jump** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, type `At H` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Cut Line 2D 2**.

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

5 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

6 In the **Expression** text field, type `r`.

7 Locate the **Coloring and Style** section. In the **Width** text field, type `2`.

8 Locate the **Legends** section. Select the **Show legends** check box.

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

10 In the table, enter the following settings:

Legends
At outlet

11 In the **Concentration Jump** toolbar, click  **Plot**.