

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.

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](#page-2-0). Here, the angular gradients are considered negligible, so an axisymmetric 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 used, 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*:

$$
K = \frac{c_2^d}{c_1^d} = \frac{c_3^p}{c_4^p}
$$
 (1)

where c_i denotes the concentration of the contaminant (SI unit: mol/m³). 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 axisymmetric 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:

Results and Discussion

The surface plot in [Figure 6](#page-6-0) 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](#page-7-0). 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 (black) show the total flux with arrows positioned using a fixed time interval. The arrow line (gray) shows the stationary velocity field.

Concentration jumps arise at the boundaries between the domains. This is shown in [Figure 8](#page-8-0) 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

Modeling Instructions

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

NEW

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

MODEL WIZARD

- **1** In the **Model Wizard** window, click **2D 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 \rightarrow 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)

- In the **Geometry** toolbar, click **Rectangle**.
- In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
- In the **Width** text field, type Rhf.
- In the **Height** text field, type H.
- Click **Build Selected**.
- **6** Click the **A^{** \leftarrow **} Zoom Extents** button in the **Graphics** toolbar.

Rectangle 2 (r2)

- In the **Geometry** toolbar, click **Rectangle**.
- In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
- In the **Width** text field, type Lm.
- In the **Height** text field, type H.
- Locate the **Position** section. In the **r** text field, type Rhf.
- Click **Build Selected**.
- **7** Click the $\left(\frac{1}{2} \right)$ **Zoom Extents** button in the **Graphics** toolbar.

Rectangle 3 (r3)

- In the **Geometry** toolbar, click **Rectangle**.
- In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
- In the **Width** text field, type Lpc.
- In the **Height** text field, type H.
- Locate the **Position** section. In the **r** text field, type Rhf+Lm.
- Click **Build Selected**.
- **7** Click the $\left(\frac{1}{x+1}\right)$ **Zoom Extents** button in the **Graphics** toolbar.

Form Union (fin)

- In the **Model Builder** window, click **Form Union (fin)**.
- In the **Settings** window for **Form Union/Assembly**, click **Build Selected**.

Dialysate and Permeate

- **1** In the **Geometry** toolbar, click **C**₁ Selections and choose Explicit Selection.
- In the **Settings** window for **Explicit Selection**, type Dialysate and Permeate in the **Label** text field.
- 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 **Fluid 1**.
- **2** In the **Settings** window for **Fluid**, 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 **Fluid**.
- **2** Select Domain 2 only.
- **3** In the **Settings** window for **Fluid**, 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 $\texttt{c0}_\text{d}$ tia.
- **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 co_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 dialysatemembrane 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**.

Select Boundary 7 only.

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

- In the **Settings** window for **Partition Condition**, locate the **Partition Condition** section.
- Find the **Boundary normal** subsection. Select the **Reverse direction** checkbox.
- **5** In the K_c text field, type K.

ADD MATERIAL

- In the **Materials** toolbar, click **Add Material** to open the **Add Material** window.
- Go to the **Add Material** window.
- In the tree, select **Liquids and Gases** > **Liquids** > **Water**.
- Click the **Add to Component** button in the window toolbar.
- In the **Materials** toolbar, click **Add Material** to close the **Add Material** window.

LAMINAR FLOW (SPF)

- In the **Settings** window for **Laminar Flow**, locate the **Domain Selection** section.
- From the **Selection** list, choose **Dialysate and Permeate**.

Inlet 1

- In the **Physics** toolbar, click **Boundaries** and choose **Inlet**.
- Select Boundary 2 only.
- In the **Settings** window for **Inlet**, locate the **Boundary Condition** section.
- 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

- In the **Physics** toolbar, click **Boundaries** and choose **Inlet**.
- Select Boundary 8 only.
- In the **Settings** window for **Inlet**, locate the **Boundary Condition** section.
- 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

- In the **Physics** toolbar, click **Boundaries** and choose **Outlet**.
- Select Boundaries 3 and 9 only.
- In the **Settings** window for **Outlet**, locate the **Pressure Conditions** section.

Select the **Normal flow** checkbox.

MESH 1

Mapped 1 In the Mesh toolbar, click **Mapped**.

Distribution 1

- Right-click **Mapped 1** and choose **Distribution**.
- Select Boundaries 1, 4, 7, and 10 only.
- In the **Settings** window for **Distribution**, locate the **Distribution** section.
- From the **Distribution type** list, choose **Predefined**.
- In the **Number of elements** text field, type 250.
- In the **Element ratio** text field, type 25.

Distribution 2

- In the **Model Builder** window, right-click **Mapped 1** and choose **Distribution**.
- Select Boundaries 5 and 6 only.
- In the **Settings** window for **Distribution**, locate the **Distribution** section.
- From the **Distribution type** list, choose **Predefined**.
- In the **Number of elements** text field, type 7.
- In the **Element ratio** text field, type 2.
- Select the **Symmetric distribution** checkbox.

Distribution 3

- Right-click **Mapped 1** and choose **Distribution**.
- Select Boundaries 2 and 3 only.
- In the **Settings** window for **Distribution**, locate the **Distribution** section.
- From the **Distribution type** list, choose **Predefined**.
- In the **Number of elements** text field, type 20.
- In the **Element ratio** text field, type 2.

Distribution 4

- Right-click **Mapped 1** and choose **Distribution**.
- Select Boundary 9 only.
- **3** Click the $\left(\frac{1}{x} \right)$ **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** checkbox.

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

STUDY 1

Laminar Flow

- **1** In the **Model Builder** window, under **Study 1** click **Step 1: Stationary**.
- **2** In the **Settings** window for **Stationary**, type Laminar Flow in the **Label** text field.
- **3** Locate the **Physics and Variables Selection** section. In the **Solve for** column of the table, under **Component 1 (comp1)**, clear the checkbox for **Transport of Diluted Species (tds)**.

Transport of Diluted Species

- **1** In the Study toolbar, click \mathcal{F} Study Steps and choose Stationary > Stationary.
- **2** In the **Settings** window for **Stationary**, type Transport of Diluted Species in the **Label** text field.
- **3** Locate the **Physics and Variables Selection** section. In the **Solve for** column of the table, under **Component 1 (comp1)**, clear the checkbox for **Laminar Flow (spf)**.

Concentration (tds)

- **1** In the **Study** toolbar, click **Compute**.
- **2** Click the **Show More Options** button in the **Model Builder** toolbar.
- **3** In the **Show More Options** dialog, in the tree, select the checkbox for the node **Results** > **Views**.
- **4** 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.
- From the **View scale** list, choose **Manual**.
- In the **x scale** text field, type 25.
- Click the **A Zoom Extents** button in the **Graphics** toolbar.

Concentration (tds)

- In the **Model Builder** window, under **Results** click **Concentration (tds)**.
- In the **Settings** window for **2D Plot Group**, locate the **Plot Settings** section.
- From the **View** list, choose **View 2D 2**.
- In the **Concentration (tds)** toolbar, click **Plot**.

Surface 1

- In the **Model Builder** window, expand the **Concentration (tds)** node, then click **Surface 1**.
- In the **Settings** window for **Surface**, locate the **Coloring and Style** section.
- From the **Color table** list, choose **JupiterAuroraBorealis**.
- **4** Click the $\left|\mathbf{I}\right|$ **Zoom Extents** button in the **Graphics** toolbar.

Arrow Surface 1

In the **Model Builder** window, right-click **Arrow Surface 1** and choose **Disable**.

Concentration (tds)

In the **Concentration (tds)** toolbar, click **Streamline**.

Streamline 1

- In the **Settings** window for **Streamline**, locate the **Streamline Positioning** section.
- From the **Positioning** list, choose **On selected boundaries**.
- In the **Number** text field, type 13.
- Locate the **Selection** section. Click to select the **Activate Selection** toggle button.
- Select Boundary 2 only.
- Locate the **Coloring and Style** section. Find the **Point style** subsection. From the **Type** list, choose **Arrow**.
- From the **Arrow distribution** list, choose **Equal time**.
- From the **Arrow length** list, choose **Normalized**.
- Select the **Scale factor** checkbox. In the associated text field, type 2.
- From the **Color** list, choose **Custom**.
- **11** On Windows, click the colored bar underneath, or $-$ if you are running the crossplatform desktop — the **Color** button.

Click **Define custom colors**.

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

Click **Add to custom colors**.

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

- In the **Model Builder** window, right-click **Arrow Line 1** and choose **Selection**.
- Select Boundaries 2 and 8 only.

Arrow Line 1

- In the **Model Builder** window, click **Arrow Line 1**.
- 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**.
- Locate the **Arrow Positioning** section. In the **Number of arrows** text field, type 39.
- Locate the **Coloring and Style** section.
- Select the **Scale factor** checkbox. In the associated text field, type 1400.
- In the **Concentration (tds)** toolbar, click **Plot**.

Concentration 2D Revolution

- In the **Model Builder** window, under **Results** click **Concentration, 3D (tds)**.
- In the **Settings** window for **3D Plot Group**, type Concentration 2D Revolution in the **Label** text field.
- Locate the **Plot Settings** section. Clear the **Plot dataset edges** checkbox.

Surface 1

- In the **Model Builder** window, expand the **Concentration 2D Revolution** node, then click **Surface 1**.
- In the **Settings** window for **Surface**, locate the **Coloring and Style** section.
- From the **Color table** list, choose **JupiterAuroraBorealis**.

Concentration 2D Revolution

- In the **Model Builder** window, click **Concentration 2D Revolution**.
- In the **Concentration 2D Revolution** toolbar, click **Plot**.
- **3** Click the $\left|\frac{1}{x}\right|$ **Zoom Extents** button in the **Graphics** toolbar.

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

Surface

- In the **Model Builder** window, expand the **Velocity (spf)** node, then click **Surface**.
- In the **Settings** window for **Surface**, locate the **Coloring and Style** section.
- From the **Color table** list, choose **Wave**.

Visualize the pressure contours in the dialysate and permeate separately.

Selection 1

- In the **Model Builder** window, expand the **Pressure (spf)** node.
- Right-click **Contour** and choose **Selection**.
- Select Domain 3 only.

Contour

- In the **Model Builder** window, click **Contour**.
- In the **Settings** window for **Contour**, locate the **Levels** section.
- In the **Total levels** text field, type 20.

Contour 2

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

Selection 1

- In the **Model Builder** window, expand the **Contour 2** node, then click **Selection 1**.
- In the **Settings** window for **Selection**, locate the **Selection** section.
- Click **Clear Selection**.
- Select Domain 1 only.
- In the **Pressure (spf)** toolbar, click **Plot**.
- Click the **Az Zoom Extents** button in the **Graphics** toolbar.

Velocity 2D Revolution

- In the **Model Builder** window, under **Results** click **Velocity, 3D (spf)**.
- In the **Settings** window for **3D Plot Group**, type Velocity 2D Revolution in the **Label** text field.

Surface

- In the **Model Builder** window, expand the **Velocity 2D Revolution** node, then click **Surface**.
- In the **Settings** window for **Surface**, locate the **Coloring and Style** section.
- 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](#page-8-0).

Cut Line 2D 1

- In the **Results** toolbar, click **Cut Line 2D**.
- In the **Settings** window for **Cut Line 2D**, locate the **Line Data** section.
- In row **Point 1**, set **z** to H/2.
- In row **Point 2**, set **r** to Rhf+Lm+Lpc and **z** to H/2.

Cut Line 2D 2

- In the **Results** toolbar, click **Cut Line 2D**.
- In the **Settings** window for **Cut Line 2D**, locate the **Line Data** section.
- In row **Point 1**, set **z** to H.
- In row **Point 2**, set **r** to Rhf+Lm+Lpc and **z** to H.

Concentration Jump

- In the **Results** toolbar, click **1D Plot Group**.
- In the **Settings** window for **1D Plot Group**, type Concentration Jump in the **Label** text field.

At H/2

- Right-click **Concentration Jump** and choose **Line Graph**.
- In the **Settings** window for **Line Graph**, type At H/2 in the **Label** text field.
- Locate the **Data** section. From the **Dataset** list, choose **Cut Line 2D 1**.
- Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.
- In the **Expression** text field, type r.
- Click to expand the **Coloring and Style** section. From the **Width** list, choose **2**.
- Click to expand the **Legends** section. Select the **Show legends** checkbox.
- From the **Legends** list, choose **Manual**.
- In the table, enter the following settings:

Legends

At half fiber length

At H

- In the **Model Builder** window, right-click **Concentration Jump** and choose **Line Graph**.
- In the **Settings** window for **Line Graph**, type At H in the **Label** text field.
- Locate the **Data** section. From the **Dataset** list, choose **Cut Line 2D 2**.
- Click to expand the **Title** section. From the **Title type** list, choose **None**.
- Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.
- In the **Expression** text field, type r.
- Locate the **Coloring and Style** section. From the **Width** list, choose **2**.
- Locate the **Legends** section. Select the **Show legends** checkbox.
- From the **Legends** list, choose **Manual**.

In the table, enter the following settings:

Legends

At outlet

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