COMSOL MULTIPHYSICS®

Separation through Dialysis

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Separation through Dialysis

Introduction

Dialysis is a frequently used membrane separation process. An important application is hemodialysis, where membranes are used as artificial kidneys for people suffering from renal failure. Other applications include the recovery of caustic colloidal hemicellulose during viscose manufacturing, and 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 obtained as a result of differences in diffusion rates across the membrane arising from differences in molecular size and solubility.

This example looks at 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. A large number of hollow fibers are assembled in a module where the dialysate flows on the fibers' insides while the permeate flows on their outsides in a co-current manner. The contaminant diffuses through the fiber walls to the permeate side due to a concentration gradient, whereas species with a higher molecular weight, those you want kept in the dialysate, are retained due to their low solubility and diffusivity in the membrane.

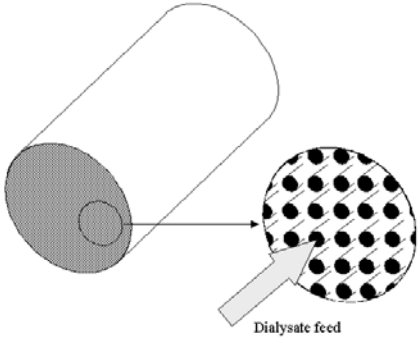

Figure 1: Diagram of the hollow fiber module.

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, which flows laminarly in the same direction as the dialysate. This example thus models three separate phases: the dialysate, the membrane, and the permeate. The model domain appears in Figure 2. Assume there are no angular gradients, so you can thus use an axisymmetrical approximation.

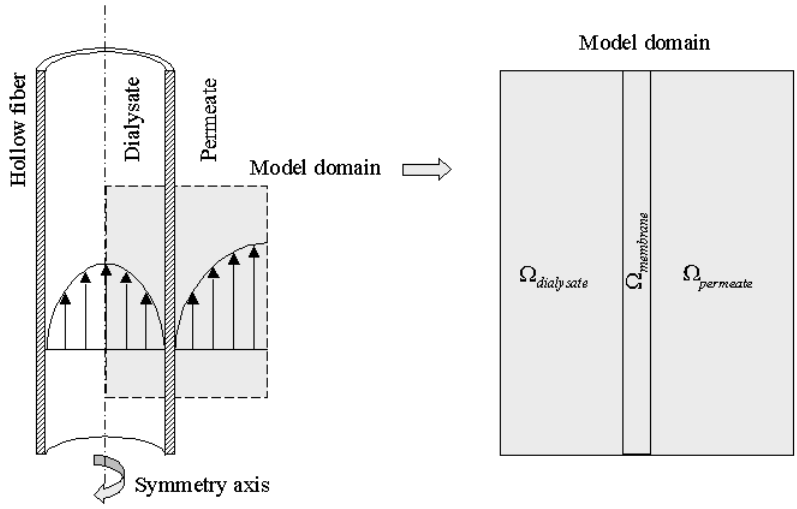

Figure 2: Diagram of the dialysis fiber.

The contaminant is transported by diffusion and convection in the two liquid phases, whereas diffusion is the only transport mechanism in the membrane phase. You can formulate the following mass transport equations to describe the system:

$$\begin{aligned} &\nabla \cdot (-D\nabla c_1 + c_1\mathbf{u}) = 0 && \text{in } \Omega_{\text{dialysate}} \\ &\nabla \cdot (-D_{\text{m}}\nabla c_2) = 0 && \text{in } \Omega_{\text{membrane}} \\ &\nabla \cdot (-D\nabla c_3 + c_3\mathbf{u}) = 0 && \text{in } \Omega_{\text{permeate}} \end{aligned} \tag{1}$$

where c_i denotes the concentration of the contaminant (mol/m^3) in the respective phases, D denotes the diffusion coefficient (m^2/s) in the liquid phases, and D_{m} is the

diffusion coefficient in the membrane, while **u** denotes the velocity (m/s) in the respective liquid phase.

The fiber is 75 times longer than its radial dimension, in this case 0.28 mm in radius and 21 mm in length. To avoid excessive amounts of elements and nodes you must scale the problem. Therefore introduce a new scaled z-coordinate, $\hat{z}$, and a corresponding differential for the mass transports:

$$\begin{aligned} \hat{z} &= \frac{z}{\mathrm{scale}} \\ dz &= \mathrm{scale} \cdot d\hat{z} \end{aligned} \tag{2}$$

In the mass-transport equations, c is differentiated twice in the diffusion term, which implies that the diffusive flux vector's z-component must be multiplied by $(1/\mathrm{scale})^2$. The convective component is only differentiated once, and therefore must be multiplied by $1/\mathrm{scale}$. You can introduce the scaling of the diffusive part of the flux as an anisotropic diffusion coefficient where the diffusion in the z direction is scaled by the factor $(1/\mathrm{scale})^2$. This gives the following diffusion-coefficient matrix:

$$\bar{D} = \begin{bmatrix} D & 0 \\ 0 & \dfrac{D}{\mathrm{scale}^2} \end{bmatrix} \tag{3}$$

To obtain the convective part of the flux, assume fully developed laminar flow both inside and outside the hollow fiber. This allows you to introduce the velocity distributions analytically. For the interior, this example uses the following velocity distribution (Ref. 2):

$$v_z^{\mathrm{dialysate}} = v_{\max}\left[1 - \left(\frac{r}{R_1}\right)^2\right] \tag{4}$$

where v_z is the axial component of the velocity, $v_{\max}$ is the maximum velocity in the axial direction, r represents the radial coordinate, and R_1 equals the inner radius of the hollow fiber. The velocity vector must be multiplied by $1/\mathrm{scale}$ to account for the new scaled z-coordinate.

Outside the fiber the velocity profile is more complicated. You can draw a hexagonal-shaped unit cell of the fiber assembly (Figure 3):

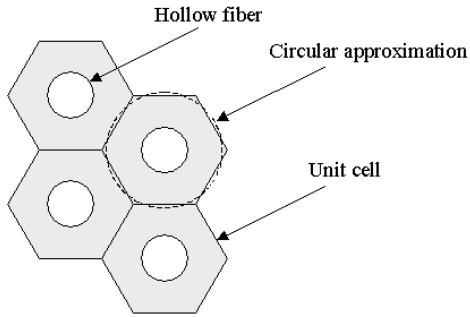

Figure 3: Hexagonal-shaped unit cell of the fiber assembly.

By approximating the hexagon with a circle, you can assume that the circle indicates the permeate's position of maximum velocity in the axial direction. In order to characterize the flow profile, the model twice integrates a momentum balance over a thin cylindrical shell (Ref. 2) to eventually get the following analytical expression for the permeate velocity distribution:

$$v_{\hat{z}}^{\text{permeate}} = A \cdot \left[r^2 - R_2^2 - 2 \cdot R_3^2 \cdot \ln\left(\frac{r}{R_2}\right) \right] \tag{5}$$

Here A (1/(m·s)) is a constant defined by

$$A = -\frac{P_0 - P_L}{4\eta L \cdot \text{scale}} \tag{6}$$

In these equations, R_2 and R_3 are the radial coordinates of the outer fiber wall and the approximated circle, respectively, η (Pa·s) is the permeate's dynamic viscosity, and $P_0 - P_L$ (Pa) represents the pressure drop over a length L.

The contaminant must dissolve into the membrane phase in order to be transported through it. The interface conditions between the liquid and membrane phases for the concentration are described by the dimensionless partition coefficient, K:

$$K = \frac{c_2^{\text{d}}}{c_1^{\text{d}}} = \frac{c_2^{\text{p}}}{c_3^{\text{p}}} \tag{7}$$

Figure 4 shows a schematic concentration profile. Note that there are discontinuities in the concentration profile at the phase boundaries.

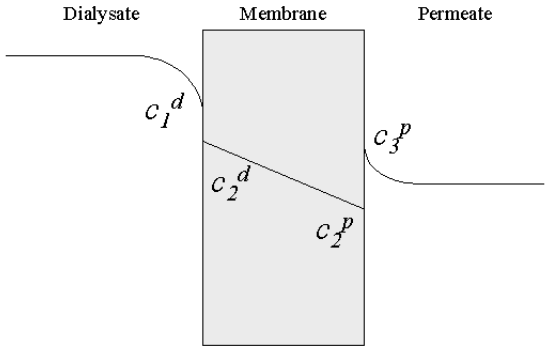

Figure 4: Diagram of the concentration profile across the membrane (see Equation 7).

To obtain a well-posed problem, you must define an appropriate set of boundary conditions; for the relevant notation, see Figure 5.

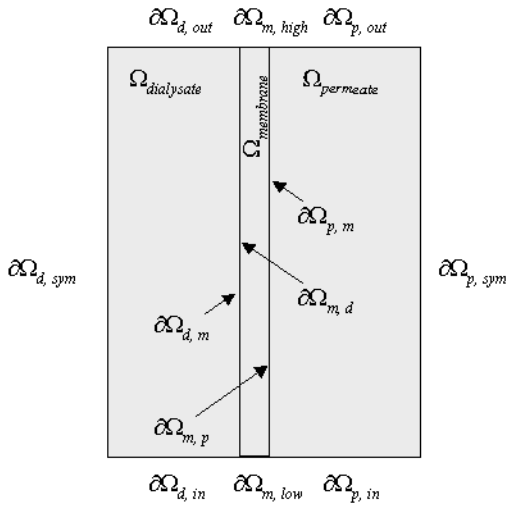

Figure 5: Boundaries and boundary labels for the modeled system.

At the inlet to the model domain, define concentration conditions as:

$$c_1 = c_0 \qquad \text{at } \partial\Omega_{\text{d, in}}$$
$$c_3 = 0 \qquad \text{at } \partial\Omega_{\text{p, in}} \tag{8}$$

At the outlet, assume that the convective contribution to the mass transport is much larger than the diffusive contribution:

$$(-D\nabla c_i + c_i\mathbf{u})\cdot\mathbf{n} = c_i\mathbf{u}\cdot\mathbf{n} \quad \text{at } \partial\Omega_{\text{d,out}} \text{ and } \partial\Omega_{\text{p, out}} \tag{9}$$

Here $\mathbf{n}$ is the normal unit vector to the respective boundary. Further, assume that you have no transport over the symmetry boundaries:

$$(-D\nabla c_i + c_i\mathbf{u})\cdot\mathbf{n} = 0 \quad \text{at } \partial\Omega_{\text{d, sym}} \text{ and } \partial\Omega_{\text{p, sym}} \tag{10}$$

Also assume symmetry at the horizontal boundaries of the membrane:

$$(-D_{\text{m}}\nabla c_2)\cdot\mathbf{n} = 0 \quad \text{at } \partial\Omega_{\text{m, high}} \text{ and } \partial\Omega_{\text{m, low}} \tag{11}$$

You can verify this assumption after solving the model by studying the very small vertical concentration gradient in the membrane.

MODEL DATA

The input data used in this model are listed in the following table:

PROPERTY	VALUE	DESCRIPTION
D	10^{-9} m^2/s	Diffusion coefficient, liquid phases
D_{m}	10^{-9} m^2/s	Diffusion coefficient, membrane
R_1	0.2 mm	Inner radius, hollow fiber
R_2	0.28 mm	Outer radius, hollow fiber
R_3	0.7 mm	Approximative radius, unit cell
v_{max}	1 mm/s	Maximum velocity, dialysate
A	$-2\cdot10^{-3}$ 1/(m·s)	Permeate velocity prefactor
K	0.7	Partition coefficient
c_0	1 M	Inlet concentration, dialysate
M	10^4 m/s	Stiff-spring velocity
scale	7	Axial coordinate scale factor

Results

The surface plot in Figure 6 visualizes the concentration distribution throughout the three model domains: the dialysate region inside the hollow fiber on the left side, the membrane in the middle, and the permeate to the right.

As the plot shows, the concentration inside the hollow fiber decreases markedly over the first 10 mm from the inlet. After this the separation process is less effective. You can also see from the plot that it takes almost 4 mm before the concentration in the core part of the fiber is influenced by the filtration process. The figure further shows the developing diffusion layers on both sides of the fiber wall.

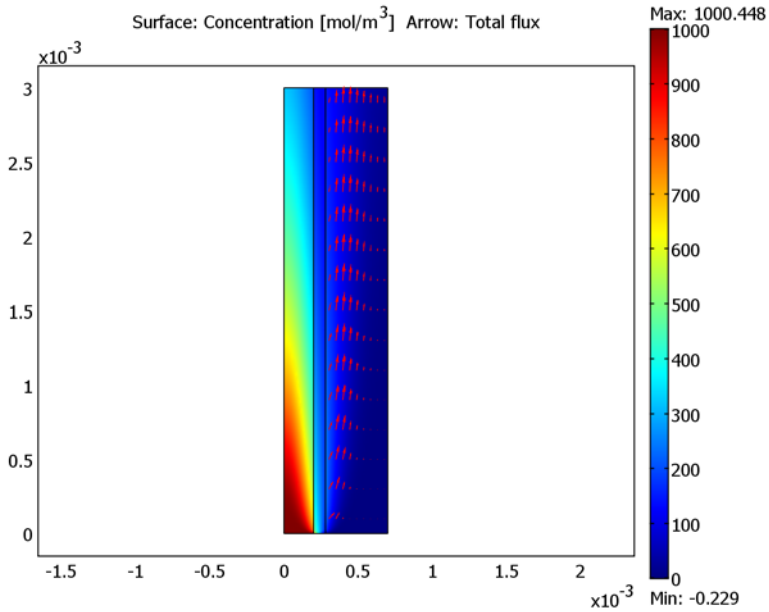

Figure 6: Concentration and flux in the three subdomains.

The figure also shows the concentration jump that arises at the boundary between the dialysate and the membrane. Further, the maximum concentration in the permeate occurs a few millimeters downstream from the inlet. If there is a risk of scaling on the fiber's outer surface due to high concentration of filtrated species, it is largest at the location of this maximum.

Note that this example models only a short piece at the hollow fiber's inlet end. Using a larger scale factor you can model the fiber's entire length.

Modeling in COMSOL Multiphysics

Because there are discontinuities in the concentration profile at the boundaries between liquid and membrane phases, you must use three separate variables to describe the concentration in the respective phases. To get continuous flux over the phase boundaries, apply a special type of boundary condition using the stiff-spring method. Instead of defining Dirichlet concentration conditions according to the partition coefficient K, which would destroy the continuity of the flux, you can define continuous flux conditions that, at the same time, force the concentrations to the desired values:

$$\begin{aligned}
(-D\nabla c_1 + c_1\mathbf{u})\cdot\mathbf{n} &= M(c_2 - Kc_1) \qquad \text{at } \partial\Omega^{\mathrm{d/m}} \\
(-D_{\mathrm{m}}\nabla c_2)\cdot\mathbf{n} &= M(Kc_1 - c_2) \qquad \text{at } \partial\Omega^{\mathrm{m/d}} \\
(-D_{\mathrm{m}}\nabla c_2)\cdot\mathbf{n} &= M(Kc_3 - c_2) \qquad \text{at } \partial\Omega^{\mathrm{m/p}} \\
(-D\nabla c_3 + c_3\mathbf{u})\cdot\mathbf{n} &= M(c_2 - Kc_3) \qquad \text{at } \partial\Omega^{\mathrm{p/m}}
\end{aligned} \tag{12}$$

Here M is a (nonphysical) velocity large enough to let the concentration differences in the brackets approach zero, thereby satisfying Equation 7. These boundary conditions also give a continuous flux across the interfaces provided that M is sufficiently large.

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.