

FEMLAB[®] 3

Multiphysics Modeling

Separation through Dialysis solved with FEMLAB 3

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Separation through Dialysis

Dialysis is a frequently used membrane separation process. One important application is hemodialysis, where membranes are used as artificial kidneys for people suffering from renal failure. Other applications are recovery of caustic colloidal hemicellulose during viscose manufacturing and removal of alcohol from beer [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.

In this example, we will look 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. We will focus on the transport of the contaminant in the hollow fiber and through its wall.

The hollow fiber assembly is schematically viewed in Figure 4-11. A large number of hollow fibers are assembled together in a module where the dialysate flows on the inside of the fibers, while the permeate flows on the outside, in a co-current manner. The contaminant diffuses through the fiber walls to the permeate side due to a concentration gradient, whereas higher molecular weight species, that we want kept in the dialysate, are retained due to their low solubility and diffusivity in the membrane.

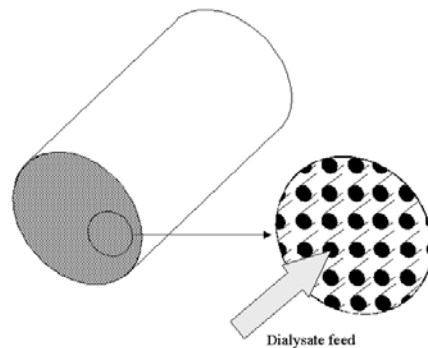


Figure 0-1: Schematic drawing of the hollow fiber module.

MODEL DEFINITION

We will model a piece of hollow fiber through which the dialysate flows with a fully developed laminar parabolic velocity profile. The fiber is surrounded by permeate, which flows laminarily in the same direction as the dialysate. We will consequently model three separate phases: the dialysate, the membrane, and the permeate. The model domain is shown in Figure 4-12. We will assume that there are no angular gradients present, and can therefore use an axisymmetrical approximation.

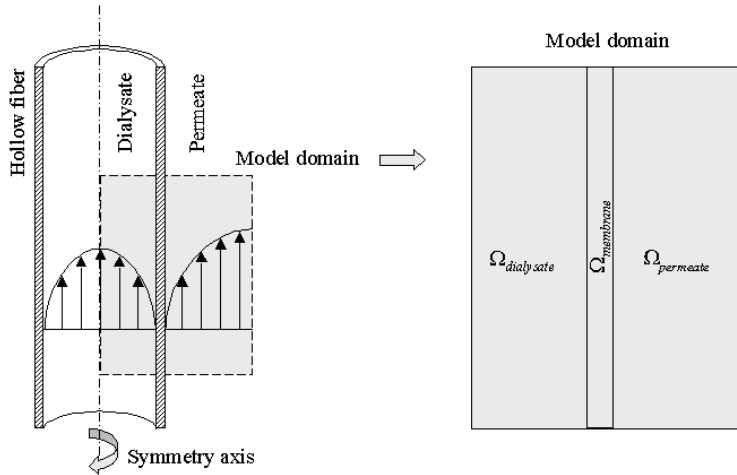


Figure 0-2: Schematic picture of the dialysis fibre

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

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

where c_i denotes the concentration of the contaminant (mol m^{-3}) in the respective phases, D the diffusion coefficient ($\text{m}^2 \text{s}^{-1}$) in the liquid phases, and D_m the diffusion coefficient in the membrane, while \mathbf{u} denotes the velocity vector 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 amount of elements and nodes, we need to scale the problem. We will therefore introduce a new scaled z -coordinate, and a new differential for the mass balances, according to Figure 4-15:

$$\begin{aligned}\hat{z} &= \frac{z}{scale} \\ dz &= scale \cdot d\hat{z}\end{aligned}\tag{0-2}$$

In the mass balances, c is differentiated twice in the diffusion term, which implies that the z -part of the diffusive flux vector has to be multiplied by $(1/scale)^2$. The convective part is only differentiated once, and has to be multiplied by $(1/scale)$. The scaling of the diffusive part of the flux can be introduced as an anisotropic diffusion coefficient where the diffusion in the z -direction is scaled by the factor $(1/scale)^2$. This gives the diffusion coefficient according to the matrix below:

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

We can obtain the convective part of the flux by assuming fully developed laminar flow both inside and outside of the hollow fiber, which allows us to introduce the velocity distributions analytically. For the interior, we use the following velocity distribution [2]:

$$v_z^{\text{dialysate}} = v_{\max} \left[1 - \left(\frac{r}{R_1} \right)^2 \right]\tag{0-4}$$

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

Outside of the fiber, the velocity profile is more complicated. We can draw a hexagonal shaped unit cell of the fiber assembly as shown in Figure 4-13:

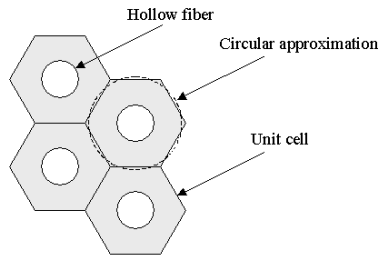


Figure 0-3: Hexagonal shaped unit cell of the fiber assembly.

If we approximate the hexagon with a circle, we can assume that the circle indicates the position of maximum velocity of the permeate in the axial direction. In order to characterize the flow profile, we integrate a momentum balance over a thin cylindrical shell twice [2], to eventually get the following analytical expression for the permeate velocity distribution:

$$v_z^{\text{permeate}} = A \cdot \left[r^2 - R_2^2 - 2 \cdot R_3^2 \cdot \ln\left(\frac{r}{R_2}\right) \right] \quad (0-5)$$

where A is a constant according to

$$A = -\frac{P_0 - P_L}{4\mu L \cdot \text{scale}} \quad (0-6)$$

R_2 and R_3 are the radial coordinates of the outer fiber wall and the approximated circle respectively, while $P_0 - P_L$ represents the pressure drop over a length L .

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

$$K = \frac{c_2^d}{c_1} = \frac{c_2^p}{c_3} \quad (0-7)$$

A schematic concentration profile is shown in Figure 4-14. Note that there are discontinuities in the concentration profile at the phase boundaries.

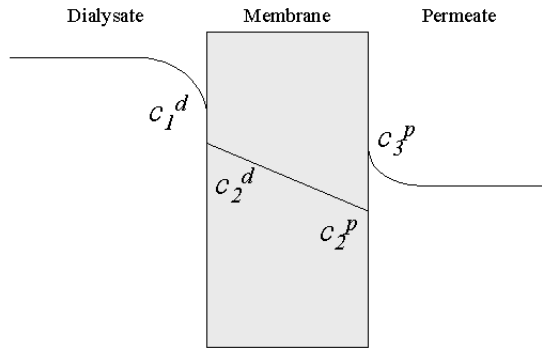


Figure 0-4: Schematic representation of the concentration profile across the membrane due to the partition coefficient, Equation 4-20.

We need to define the boundary conditions in order to obtain a well-posed problem, see Figure 4-15:

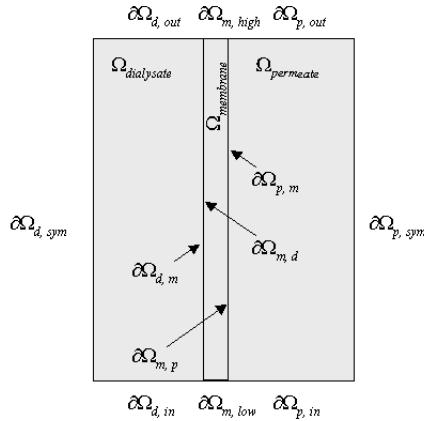


Figure 0-5: Boundaries and boundary labels for the modeled system.

At the inlet to our model domain, we define concentration conditions according to:

$$\begin{aligned} c_1 &= c_0 & \text{at } \partial\Omega_{d, \text{in}} \\ c_3 &= 0 & \text{at } \partial\Omega_{p, \text{in}} \end{aligned} \quad (0-8)$$

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

$$(-D\nabla c_i + c_i \mathbf{u}) \cdot \mathbf{n} = c_i \mathbf{u} \cdot \mathbf{n} \quad \text{at } \partial\Omega_{d,\text{out}} \text{ and } \partial\Omega_{p,\text{out}} \quad (0-9)$$

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

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

We also assume symmetry at the horizontal boundaries of the membrane:

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

This assumption can be verified when the model has been solved by studying the very small vertical concentration gradient in the membrane.

MODEL DATA

The input data used in this model is listed in Table 4-3:

TABLE 0-1: INPUT DATA

PROPERTY	VALUE
D	1e-9 m ² /s
Dm	1e-9 m ² /s
Fiber diameter	0.56 mm
Membrane thickness	0.28 mm
R1	0.2 mm
R2	0.28 mm
R3	0.7 mm
vmax, dialysate	1e-3 m/s
A	-2e-3 1/m/s
K	0.7
c10	1000 mol/m ³
M	1e4
scale	7

RESULTS

The color plot in Figure 4-16 visualizes the concentration distributions in the three model domains, the dialysate on the left-hand side, the membrane in the middle, and the permeate to the right.

We can see from the figure that the concentration inside the hollow fiber decreases markedly in the first 10 mm of the fiber. After this, the separation process is less effective. We 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 also shows the developing diffusion layers on both sides of the fiber wall.

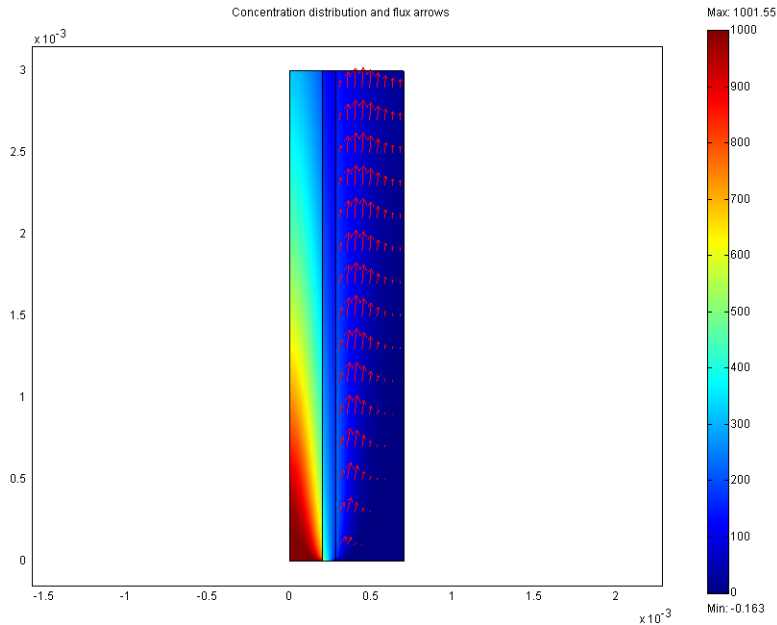


Figure 0-6: Concentration and flux in the three subdomains.

The figure also shows the concentration jump that arises at the boundary between the dialysate and the membrane. In Figure 4-16, we can also see that the maximum in concentration in the permeate takes place a few mm downstream from the inlet. If there is a risk of scaling on the outer surface of the fiber due to high concentration of filtrated species, this risk is largest at the location of this maximum.

Note that in this example, only a short piece at the inlet of the hollow fiber and surrounding permeate has been modeled. There is also a possibility to scale the problem even more, in such a way that the whole length of the fiber is modeled.

REMARKS ABOUT THE FEMLAB IMPLEMENTATION

As there will be discontinuities in the concentration profile at the boundaries between liquid and membrane phases, we will use three separate variables to describe the concentration in the respective phases. In order to get continuous flux over the phase boundaries, we will 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—we define continuous flux conditions that, at the same time, force the concentrations to the desired values:

$$\begin{aligned}(-D\nabla c_1 + c_1 \mathbf{u}) \cdot \mathbf{n} &= M(c_2 - Kc_1) && \text{at } \partial\Omega^{d/m} \\ (-D_m \nabla c_2) \cdot \mathbf{n} &= M(Kc_1 - c_2) && \text{at } \partial\Omega^{m/d} \\ (-D_m \nabla c_2) \cdot \mathbf{n} &= M(Kc_3 - c_2) && \text{at } \partial\Omega^{m/p} \\ (-D\nabla c_3 + c_3 \mathbf{u}) \cdot \mathbf{n} &= M(c_2 - Kc_3) && \text{at } \partial\Omega^{p/m}\end{aligned}\tag{0-12}$$

where M is a large enough number to let the concentration differences in the brackets approach zero. Equation 4-20 will thereby be satisfied. Note that these boundary conditions also give us continuity in flux, provided M is sufficiently large.

REFERENCES

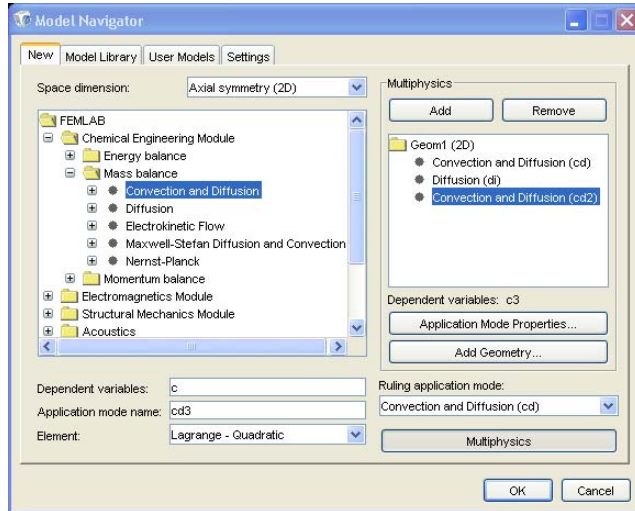
- [1] M. Mulder, *Basic Principles of Membrane Technology*. Second edition, Kluwer Academic Publishers, 1998.
- [2] R. B. Bird, W.E. Stewart and E.N. Lightfoot, *Transport Phenomena*, John Wiley & Sons, 1960.

Model Library path: Chemical_Engineering_Module/Mass_Transport/
dialysis

Modeling Using the Graphical User Interface

- 1 Start FEMLAB
- 2 In the **Model Navigator**, click the **Multiphysics** button, and set the **Space Dimension** list to **Axial symmetry (2D)**.
- 3 Choose the application mode **Chemical Engineering Module/Mass balance/Convection and Diffusion**.

- 4 Type **c1** in the **Dependent variables** edit field. Click the **Add** button. Repeat the procedure for **Chemical Engineering Module/Mass balance/Diffusion**, and name the dependent variable **c2**.
- 5 Finally, add another **Chemical Engineering/Mass balance/Convection and Diffusion**, name the variable **c3**.



OPTIONS AND SETTINGS

- 1 Define the following constants by selecting the menu item **Options>Constants**:

NAME	EXPRESSION
D	1e-9
Dm	1e-9
M	1e4
K	0.7
c0	1e3
R1	2e-4
R2	2.8e-4
R3	7e-4
v1max	1e-3
A	-2e3
scale	7

GEOMETRY MODELING

- 1 Click the **Rectangle/Square** button on the Draw toolbar and draw a rectangle of arbitrary dimension. Repeat once to get two rectangles.
- 2 Double-click on each rectangle in turn and type the below values in the corresponding edit fields.

EDIT FIELD	R1	R2
Width	2.8e-4	5e-4
Height	3e-3	3e-3
r:	0	2e-4
z:	0	0

- 3 Click the **Zoom Extents** button in the Main toolbar.

PHYSICS SETTINGS

Boundary Conditions

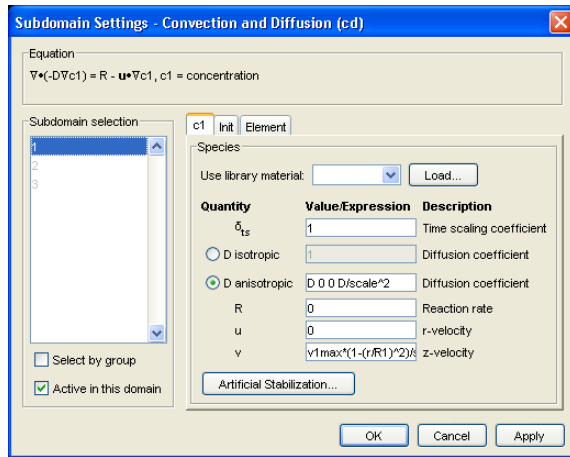
- 1 Select **I Convection and Diffusion (cd)** from the **Multiphysics** menu.
- 2 Open the **Physics/Subdomain Settings** dialog box and clear the **Active in this domain** check box for this in subdomains 2 and 3. Click **OK**.
- 3 Select the **Physics/Boundary Settings** menu item and enter the boundary conditions according to the following table:

BOUNDARY	1	2	3	4
Type	Insulation/ symmetry	Concentration	Convective flux	Flux
$c _0$		c_0		
N_0				$M*(c_2 - K*c_1)$

Subdomain Settings

- 1 Define the subdomain expression c_{all} in the **Options>Expressions>Subdomain Expressions** dialog box.
- 2 Select subdomain **1** in the **Subdomain selection** list, type c_{all} in the first **Name** edit field and c_1 in the **Expression** edit field.
- 3 Select subdomain **2** in the **Subdomain selection** list, type c_2 in the **Expression** edit field for c_{all} .
- 4 Complete by defining c_3 for subdomain **3** in the same manner.
- 5 Open the **Physics/Subdomain Settings** dialog box, and select subdomain **1**.

- Click the **D anisotropic** radio button. Place the cursor in the edit field next to this button and the diffusivity matrix will appear. Type **D** in the r-diffusivity field (upper left) and **D/scale^2** in the z-diffusivity field (lower right).
- Set **R** and **u** to 0 and **v** to $v1max*(1-(r/R1)^2)/scale$.



Initial Conditions

Click on the **Init** tab and enter 1000 in the **c1(t0)** edit field for subdomain 1.

Boundary Conditions

- Select **2 Diffusion (di)** from the **Multiphysics** menu.
- Open the **Physics/Subdomain Settings** dialog box and clear the **Active in this domain** check box in subdomains 1 and 3.
- Select **Physics>Boundary Settings** and enter the boundary conditions according to the following table:

BOUNDARY	4	5, 6	7
Type	Flux	Insulation/ Symmetry	Flux
N_0	$M*(K*c1 - c2)$		$M*(K*c3 - c2)$

- Click **OK**.

Subdomain Settings

- Open the **Physics>Subdomain Settings** dialog box, and select subdomain **2**.

- 2 Enter the anisotropic diffusivity in the same manner as in the previous application mode.

SUBDOMAIN	2
D (r-direction)	Dm
D (z-direction)	Dm / (scale ²)
R	0

Initial Conditions

The initial conditions need no action since they are defaulted to 0.

Boundary Conditions

- 1 Select **3 Convection and Diffusion (cd2)** from the **Multiphysics** menu.
- 2 Open the **Physics/Subdomain Settings** dialog box and clear the check box **Active in this domain for** subdomains 1 and 2.
- 3 Select the **Physics/Boundary Settings** menu and enter the boundary conditions according to the following table:

BOUNDARY	7	8	9	10
Type	Flux	Concentration	Convective flux	Insulation/ Symmetry
c3 ₀		0		
N ₀	M*(c2-K*c3)			

Subdomain Settings

- 1 Open the **Physics>Subdomain Settings** dialog box, and select subdomain **3**.
- 2 Enter the anisotropic diffusivity in the same manner as in the previous application modes.

SUBDOMAIN	3
D (r-direction)	D
D (z-direction)	D / (scale ²)
R	0
u	0
v	A*((r ²) - (R2 ²) - 2*(R3 ²)*log(r/R2))/scale

Initial Conditions

Click on the **Init** tab and enter 100 in the **c3(t0)** edit field for subdomain 3.

MESH GENERATION

- 1 Initialize the mesh by clicking the **Initialize Mesh** button.
- 2 Refine the mesh once by clicking the **Refine Mesh** button.

COMPUTING THE SOLUTION

- 1 Click the **Solver Parameters** button and select **Solver: Stationary nonlinear**, and **Solution form: General**.

Solve the problem by clicking on the **Solve** button.

