Created in COMSOL Multiphysics 5.3



# Separation Through Dialysis

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# 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.

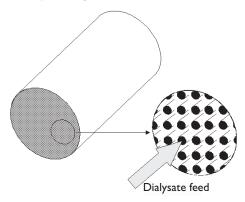


Figure 1: The hollow fiber assembly in a dialysis module.

# 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.

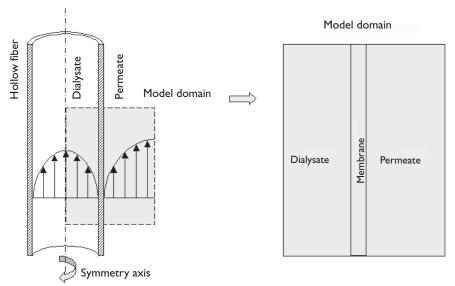
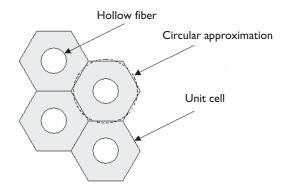


Figure 2: Illustrations of the hollow fiber setup with the dialysate and permeate, and of the model domain.



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:

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

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

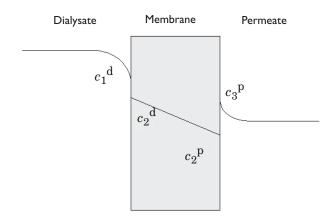


Figure 4: The concentration profile across the membrane (see Equation 1). Note that there are discontinuities in the concentration profile at the membrane boundaries.

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 boundaries are discontinuous and boundary conditions need to be set on both sides of the membrane at each liquid interface. Equation 1, set as Pointwise Constraints at the two boundaries, implements these boundary conditions in the model.

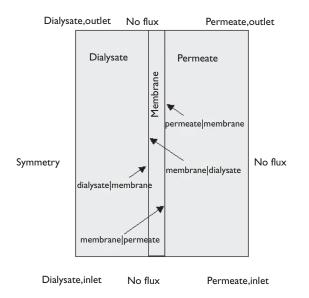


Figure 5: The boundaries accounted for in the model.

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

PROPERTY	VALUE	DESCRIPTION
D	10 <sup>-9</sup> m <sup>2</sup> /s	Diffusion coefficient, liquids
D <sub>m</sub>	10 <sup>-9</sup> m <sup>2</sup> /s	Diffusion coefficient, membrane
$R_{ m hf}$	0.2 mm	Inner radius, hollow fiber
$L_{\rm m}$	0.28 mm	Thickness, membrane
$L_{ m pc}$	0.7 mm	Width, concentric permeate channel
Η	21 mm	Length, fiber
$U_{\rm ave\_dia}$	0.5 mm/s	Average velocity, dialysate
$U_{\rm ave\_per}$	0.8 mm/s	Average velocity, permeate
Κ	0.7	Partition coefficient
$c_0$	IM	Inlet concentration, dialysate

The input data are listed in the table:

# Results

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 maximum concentration in the permeate occurs close to the outlet. If there is a risk of deposition on the fiber's outer surface due to a high concentration of filtrated

species, it is largest at the location of this maximum. The figure also shows the developing diffusion layers on both sides of the fiber wall.

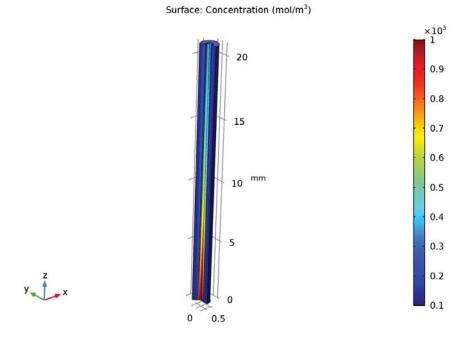


Figure 6: Concentration in the three domains as seen from the inlet of the fiber.

Concentration jumps arise at the boundaries between the domains. This is shown in Figure 7 where the concentration profile at the middle of the fiber length is plotted along the radius of the model geometry.

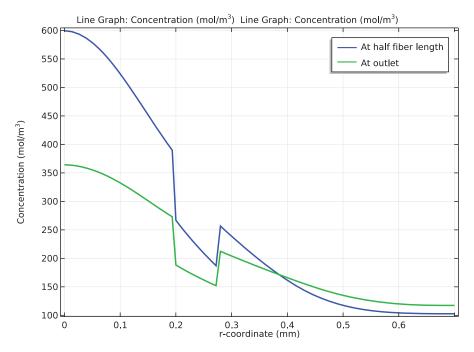


Figure 7: Concentration across the three domains at the middle of the fiber length and at the outlet.

# Modeling in COMSOL Multiphysics

Manually defined point-wise constraints are used to model the discontinuities in the concentration profile at the boundaries between the liquid and membrane phases. The constraint expressions are defined according to Equation 1.

When defining these constraints the constraint forces need to be set to ensure a continuous flux over the phase boundaries. This is done by using test() operators, operating on the dependent variables that are solved for in each domain, for example test(c1). What the test() terms in the force expressions represent depends on the partial differential equation solved for in each domain. In this model, the test() terms in the force expression on the liquid-membrane boundaries represent the diffusive flux.

# 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

- I 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 **Concentrations** table, enter the following settings:

c1

- 5 In the Select Physics tree, select Chemical Species Transport> Transport of Diluted Species (tds).
- 6 Click Add.
- 7 In the **Concentrations** table, enter the following settings:

c2

- 8 In the Select Physics tree, select Fluid Flow>Single-Phase Flow>Laminar Flow (spf).
- 9 Click Add.
- IO Click Study.

II In the Select Study tree, select Preset Studies for Selected Physics Interfaces>Stationary.

12 Click Done.

# GLOBAL DEFINITIONS

## Parameters

I On the Home toolbar, click Parameters.

Load parameters from a text-file.

- 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 I

- I In the Model Builder window, under Component I (compl) click Geometry I.
- 2 In the Settings window for Geometry, locate the Units section.
- 3 From the Length unit list, choose mm.

## Rectangle 1 (r1)

- Right-click Geometry 1 in Model Builder and I On the Geometry toolbar, click Primitives and choose Rectangle. choose 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 Right-click Rectangle I (rI) and choose Build Selected.
- 6 Click the **Zoom Extents** button on the **Graphics** toolbar.

#### Rectangle 2 (r2)

- Right-click Geometry 1 in Model Builder and I On the Geometry toolbar, click Primitives and choose Rectangle. choose 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 Right-click Rectangle 2 (r2) and choose Build Selected.
- 7 Click the **Zoom Extents** button on the **Graphics** toolbar.

# Rectangle 3 (r3)

# Right-click Geometry 1 in Model Builder and I On the Geometry toolbar, click Primitives and choose Rectangle. choose 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 Right-click Rectangle 3 (r3) and choose Build Selected.
- 7 Click the **Zoom Extents** button on the **Graphics** toolbar.

#### Form Union (fin)

In the Model Builder window, under Component I (compl)>Geometry I right-click Form Union (fin) and choose Build Selected.

Explicit Selection 1 (sell)

Right-click Geometry 1 in Model Builder

- I On the Geometry toolbar, click Selections and choose Explicit Selection. and choose Selection > 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. Select Domains 1 and 3 in the Graphics window.

#### Explicit Selection 2 (sel2)

- I On 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. Select Domain 2 in the Graphics window.

# DEFINITIONS

Variables 1

I On the Home toolbar, click Variables and choose Local Variables.

Add a common variable c\_all for all concentrations.

- 2 In the Settings window for Variables, locate the Geometric Entity Selection section.
- **3** From the **Geometric entity level** list, choose **Domain**.
- **4** From the **Selection** list, choose **Dialysate and Permeate**.
- 5 Locate the Variables section. In the table, enter the following settings:

Name	Expression	Unit	Description
c_all	c1	mol/m³	Concentration

## Variables 2

- I On the Home toolbar, click Variables and choose Local Variables.
- 2 In the Settings window for Variables, locate the Geometric Entity Selection section.
- **3** From the **Geometric entity level** list, choose **Domain**.
- 4 From the Selection list, choose Membrane.
- 5 Locate the Variables section. In the table, enter the following settings:

Name	Expression	Unit	Description
c_all	c2	mol/m³	Concentration

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

# TRANSPORT OF DILUTED SPECIES (TDS)

- I In the Model Builder window, under Component I (compl) click Transport of Diluted Species (tds).
- 2 In the Settings window for Transport of Diluted Species, type Transport of Diluted Species Dialysate and Permeate in the Label text field.
- **3** Locate the **Domain Selection** section. From the **Selection** list, choose **Dialysate and Permeate**.

# TRANSPORT OF DILUTED SPECIES - DIALYSATE AND PERMEATE (TDS)

On the Physics toolbar, click Transport of Diluted Species (tds) and choose Transport of Diluted Species - Dialysate and Permeate (tds).

## Transport Properties 1

- In the Model Builder window, expand the Component I (compl)>
   Transport of Diluted Species Dialysate and Permeate (tds) node, then click
   Transport Properties I.
- 2 In the Settings window for Transport Properties, locate the Diffusion section.
- **3** In the  $D_{c1}$  text field, type D.

## Initial Values 1

- I In the Model Builder window, under Component I (compl)>Transport of Diluted Species -Dialysate and Permeate (tds) click Initial Values I.
- 2 In the Settings window for Initial Values, locate the Initial Values section.
- **3** In the *c***1** text field, type c0\_dia.

# Initial Values 2

- Right-click Component I (compl)>Transport of Diluted Species Dialysate and Permeate (tds)>Initial Values I and choose Duplicate.
- 2 Select Domain 3 only. Change Selection to Manual and leave only Domain 3 in the Selection box.
- 3 In the Settings window for Initial Values, locate the Initial Values section.
- 4 In the c1 text field, type c0\_per.

#### Inflow I

- I On 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  $c_{0,c1}$  text field, type c0\_dia.
- 5 Locate the Boundary Condition Type section. From the list, choose Flux (Danckwerts).

## Inflow 2

- I On 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  $c_{0,c1}$  text field, type c0\_per.
- 5 Locate the Boundary Condition Type section. From the list, choose Flux (Danckwerts).

## Outflow I

- I On the Physics toolbar, click Boundaries and choose Outflow.
- **2** Select Boundaries **3** and **9** only.
- **3** In the **Model Builder** window's toolbar, click the **Show** button and select **Advanced Physics Options** in the menu.

# Pointwise Constraint I

I On the Physics toolbar, click Boundaries and choose Pointwise Constraint.

Select a pointwise boundary constraint to account for the transport between the domains.

- **2** Select Boundaries 4 and 7 only.
- 3 In the Settings window for Pointwise Constraint, locate the Pointwise Constraint section.
- 4 From the Apply reaction terms on list, choose User defined.
- 5 In the Constraint expression text field, type c2-K\*c1.
- 6 In the Constraint force expression text field, type test(c2)-test(c1).

# TRANSPORT OF DILUTED SPECIES 2 (TDS2)

- I In the Model Builder window, under Component I (compl) click Transport of Diluted Species 2 (tds2).
- 2 In the **Settings** window for **Transport of Diluted Species**, type **Transport of Diluted Species** - Membrane in the **Label** text field.
- 3 Locate the Domain Selection section. From the Selection list, choose Membrane.
- 4 Locate the Transport Mechanisms section. Clear the Convection check box.

#### TRANSPORT OF DILUTED SPECIES - MEMBRANE (TDS2)

On the Physics toolbar, click Transport of Diluted Species 2 (tds2) and choose Transport of Diluted Species - Membrane (tds2).

## Transport Properties 1

- In the Model Builder window, under Component I (compl)>Transport of Diluted Species -Membrane (tds2) click Transport Properties I.
- 2 In the Settings window for Transport Properties, locate the Diffusion section.
- **3** In the  $D_{c2}$  text field, type Dm.

## Initial Values 1

- I In the Model Builder window, under Component I (compl)>Transport of Diluted Species -Membrane (tds2) click Initial Values I.
- 2 In the Settings window for Initial Values, locate the Initial Values section.
- 3 In the c2 text field, type c0\_mem.

#### ADD MATERIAL

- I On 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 On the Home toolbar, click Add Material to close the Add Material window.

#### LAMINAR FLOW (SPF)

- I In the Model Builder window, under Component I (compl) 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.
- 4 In the Model Builder window, click Laminar Flow (spf).

# Inlet 1

- I On 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 Laminar inflow.
- 5 Locate the Laminar Inflow section. In the  $U_{\rm av}$  text field, type Uave\_dia.

#### Inlet 2

- I On 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 Laminar inflow.
- 5 Locate the Laminar Inflow section. In the  $U_{\rm av}$  text field, type Uave\_per.

# Outlet I

- I On the Physics toolbar, click Boundaries and choose Outlet.
- **2** Select Boundaries **3** and **9** only.

## MULTIPHYSICS

Flow Coupling 1 (fc1)

On the Physics toolbar, click Multiphysics and choose Global>Flow Coupling.

# MESH I

Distribution I

- I In the Model Builder window, under Component I (compl) right-click Mesh I and choose Mapped.
- 2 Right-click Mapped I and choose Distribution.
- **3** Select Boundaries 1, 4, 7, and 10 only.
- 4 In the Settings window for Distribution, locate the Distribution section.
- 5 From the Distribution properties list, choose Predefined distribution type.
- 6 In the Number of elements text field, type 250.
- 7 In the **Element ratio** text field, type 25.

# Distribution 2

I Right-click Mapped I 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 properties list, choose Predefined distribution type.
- 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

- I Right-click Mapped I 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 properties** list, choose **Predefined distribution type**.
- 5 In the Number of elements text field, type 20.
- 6 In the **Element ratio** text field, type 2.

#### Distribution 4

- I Right-click Mapped I and choose Distribution.
- 2 Select Boundary 9 only.
- 3 Click the Zoom Extents button on the Graphics toolbar.
- 4 Click the Zoom Box button on the Graphics toolbar.
- **5** Select Boundaries 8 and 9 only.
- 6 In the Settings window for Distribution, locate the Distribution section.
- 7 From the Distribution properties list, choose Predefined distribution type.
- 8 In the Number of elements text field, type 30.
- 9 In the Element ratio text field, type 3.
- **IO** Select the **Reverse direction** check box.

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

# STUDY I

## Step 1: Stationary

- I In the Model Builder window, under Study I click Step I: 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 - Dialysate and Permeate (tds) and Transport of Diluted Species - Membrane (tds2).

# Step 2: Stationary 2

- I On 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 On the Study toolbar, click Compute.

Plot the concentration distribution in Figure 6. For this axisymmetric geometry, the **Revolution 2D** data set is used.

# RESULTS

Concentration (tds2) 1

- I In the Model Builder window, under Results click Concentration (tds2) I.
- 2 In the Settings window for 3D Plot Group, type Concentration 2D Revolution All in the Label text field.

Revolution 2D 2

- I On the **Results** toolbar, click **More Data Sets** and choose **Revolution 2D**.
- 2 In the Settings window for Revolution 2D, click to expand the Revolution layers section.
- 3 Locate the Revolution Layers section. In the Start angle text field, type -90.
- 4 In the **Revolution angle** text field, type 225.

Concentration 2D Revolution - All

- I In the Model Builder window, expand the Results>Concentration 2D Revolution All node, then click Concentration 2D Revolution All.
- 2 In the Settings window for 3D Plot Group, locate the Data section.
- 3 From the Data set list, choose Revolution 2D 2.

#### Surface

- I In the Model Builder window, under Results>Concentration 2D Revolution All click Surface.
- 2 In the Settings window for Surface, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Model>Component I>Definitions> Variables>c\_all - Concentration.

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

# Concentration 2D Revolution - All

- I Click the **Zoom Extents** button on the **Graphics** toolbar.
- 2 On the Concentration 2D Revolution All toolbar, click Plot.

#### Velocity (spf) 1

- I In the Model Builder window, expand the Concentration 2D Revolution All node, then click Results>Velocity (spf) I.
- 2 In the Settings window for 3D Plot Group, locate the Data section.
- 3 From the Data set list, choose Revolution 2D 2.
- 4 On the Velocity (spf) I toolbar, click Plot.

Create cut lines at two locations along the fiber length to illustrate the concentration jump between the domains in Figure 7.

Cut Line 2D I

- I On 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 I, 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

- I On 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 I**, set **Z** to H.
- 4 In row **Point 2**, set **R** to Rhf+Lm+Lpc and **z** to H.

#### ID Plot Group 8

- I On the **Results** toolbar, click **ID Plot Group**.
- 2 In the Settings window for ID Plot Group, type Concentration Jump in the Label text field.

Line Graph I

- I 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 Data set list, choose Cut Line 2D I.
- **4** Locate the **y-Axis Data** section. In the **Expression** text field, type c\_all.
- 5 Locate the x-Axis Data section. From the Parameter list, choose Expression.

- 6 In the **Expression** text field, type r.
- 7 Click to expand the **Coloring and style** section. Locate the **Coloring and Style** section. In the **Width** text field, type 2.
- 8 Click to expand the Legends section. Select the Show legends check box.
- 9 From the Legends list, choose Manual.
- **IO** In the table, enter the following settings:

# Legends

## At half fiber length

## Line Graph 2

- I Right-click Results>Concentration Jump>At H/2 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 Data set list, choose Cut Line 2D 2.
- 4 Locate the y-Axis Data section. In the Expression text field, type c\_all.
- 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.
- **IO** In the table, enter the following settings:

# Legends

At outlet

II On the Concentration Jump toolbar, click Plot.

Fix the name of all plot groups.

# Concentration (tds)

- I In the Model Builder window, under Results click Concentration (tds).
- 2 In the Settings window for 2D Plot Group, type Concentration Surface Dialysate and Permeate in the Label text field.

#### Concentration (tds) 1

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

2 In the Settings window for 3D Plot Group, type Concentration 2D revolution - Dialysate and Permeate in the Label text field.

Concentration (tds2)

- I In the Model Builder window, under Results click Concentration (tds2).
- 2 In the Settings window for 2D Plot Group, type Concentration Surface Membrane in the Label text field.

Velocity (spf)

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

Velocity (spf) 1

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