

## Taylor Dispersion

Created by Robert P. Hesketh, Chemical Engineering, Rowan University Fall 2005

In this problem you will simulate a tubular reactor with fluid flowing in laminar flow.

The governing equations for this problem can be derived from a shell balance on a ring shaped element in the cylindrical geometry. The resulting equation is

$$\frac{\partial C_A}{\partial t} = -\frac{\partial N_{Az}}{\partial z} - \frac{\partial(rN_{Ar})}{r \partial r} + r_A \quad (1)$$

For cylindrical coordinates  $r, z$  the following flux equations for convective and diffusive fluxes in the  $z$  and  $r$  directions are applicable:

$$N_{Az} = j_{Az} + y_A \sum N_i = -D_{AB} \frac{\partial C_A}{\partial z} + C_A u_z \quad (2)$$

$$N_{Ar} = j_{Ar} + y_A \sum N_i = -D_{AB} \frac{\partial C_A}{\partial r} + C_A u_r \quad (3)$$

Equation 3 can be simplified by eliminating the velocity term in the radial direction. Next substitute equations 2 and 3 into equation 1 to obtain

$$\frac{\partial C_A}{\partial t} = -\frac{\partial}{\partial z} \left( -D_{AB} \frac{\partial C_A}{\partial z} + C_A u_z \right) - \frac{\partial}{r \partial r} \left( -D_{AB} r \frac{\partial C_A}{\partial r} \right) + r_A \quad (4)$$

At steady state and assuming constant velocity in the  $z$  direction yields the following equation

$$u_z \frac{\partial C_A}{\partial z} = D_{AB} \frac{\partial^2 C_A}{\partial z^2} + D_{AB} \frac{\partial}{r \partial r} \left( r \frac{\partial C_A}{\partial r} \right) + r_A \quad (5)$$

Notice that if the diffusive flux in equation 5 is neglected then the familiar plug flow reactor equation results

$$u_z \frac{\partial C_A}{\partial z} = r_A \quad (6)$$

In this tutorial we will compare the effect of diffusion for a reactor with fluid in laminar flow.

You will start with a plug flow model and then compare this to the following

Base Case: Plug Flow

1. Laminar flow – no diffusion
2. Laminar flow – with diffusion using several diffusion coefficients and several velocities.

I suggest trying the following conditions:

$u$ (m/s)	$D_{AB}$ (m <sup>2</sup> /s)	Re	$Pe = D_{AB}/(uD_t)$
0.02	2.69E-04	7.623	0.530
0.2	2.69E-04	76.230	0.053
2	2.69E-04	762.305	0.005
0.02	2.69E-05	7.623	0.053
0.02	2.69E-06	7.623	0.005

We will look at a gas phase reaction at 700 K and assume that the density is 0.503 kg/m<sup>3</sup> and viscosity is 3.33×10<sup>-5</sup> kg/(m s). A typical diffusion coefficient for this temperature is 2.69×10<sup>-4</sup> m<sup>2</sup>/s. Assume that the reaction is first order with a reaction rate constant of 0.14 s<sup>-1</sup>.

## Modeling Using the Graphical User Interface

1. Open FEMLAB.
2. Select **axial symmetry (2D)** from the **Space dimension** list.
3. Select the application mode **Chemical Engineering Module>Mass balance>Convection and Diffusion (steady-state)**.
4. Click the **Multiphysics** button and click the **Add** button to add the application mode to the model and then **OK**.

## OPTIONS AND SETTINGS

1. Enter the following variable names in the **Constants** dialog box under the **Options** menu.

Name	Expression	Value
krxn	0.14	0.14
CA0	0.002	0.002
Diff	2.69e-4	2.69e-4
R	0.0127	0.0127
uavg	0.02	0.02
rho	0.503	0.503
eta	3.332e-5	3.332e-5

## GEOMETRY MODELING

1. Make pipe with length 0.1 m and radius 0.0127 m.  
You can do this by adding a rectangle.
2. Click the **Zoom Extents** button.

## PHYSICS SETTINGS

Open the **Expressions** dialog box from the **Options>Expressions** menu, and enter the following variable names and expressions:

Name	Expression
rA	-krxn*c
uin	2*uavg*(1-(r/R)^2)

## Boundary Conditions

- a) Specify the boundary at  $r=0$  as a symmetry axis.
- b) The wall at  $r=R$  is an Insulated boundary
- c) The inlet is a concentration boundary with uniform concentration across the cross-section of CA0.
- d) The outlet is specified as a Convective Flux boundary condition.

2) Click <b>OK</b> .	Boundary	1, 4	2	3
	Type	Insulation/Symmetry	Concentration	Convective flux
	Concentration (c0)	0	CA0	0

## Subdomain Settings

1. For the plug flow model enter material properties according to the following table in all the subdomains in the **Subdomain Settings** dialog box under the **Physics** menu:

Subdomain	1
Diffusion coefficient (D)	0
Reaction rate (R)	rA
Time-scaling coefficient (Dts)	1
r-velocity (u)	0
z-velocity (v)	uavg

2. Switch to the **Init** tab and enter uavg for the  $\mathbf{v}(\mathbf{t}_0)$  initial value. We have not done this in the past, but this will help with the giving the solver an initial value to start the solution.
3. Click **OK**.

Subdomain initial value 1  
Concentration, c (c) CA0

## MESH GENERATION

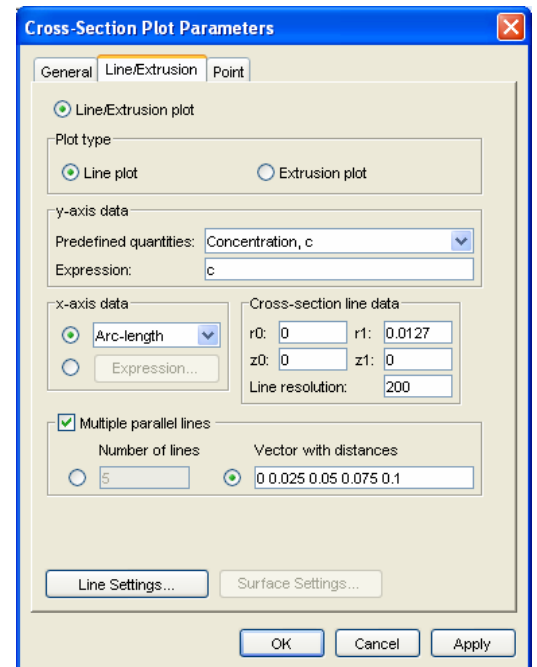
1. Select **Mesh Parameters** from the **Mesh** menu and select **Fine** in the **Predefined mesh sizes** list.
2. Click **OK**.
3. Click **Initialize Mesh** in the Main toolbar.
4. Refine the mesh once more. You may want to return to this menu to refine your mesh in the region in which the concentration is changing. Warning don't make it too fine or the computer will run out of memory.

## COMPUTING THE SOLUTION –

Click the **Solve** button in the Main toolbar to solve the problem.

## POSTPROCESSING AND VISUALIZATION

- 1) Capture the Surface plot of concentration
- 2) Make a cross section plot of the concentration profile at the axial positions of 0 m, 0.025 m, 0.05 m, 0.075 m and 0.1 m.



## PAMAMETRIC STUDIES

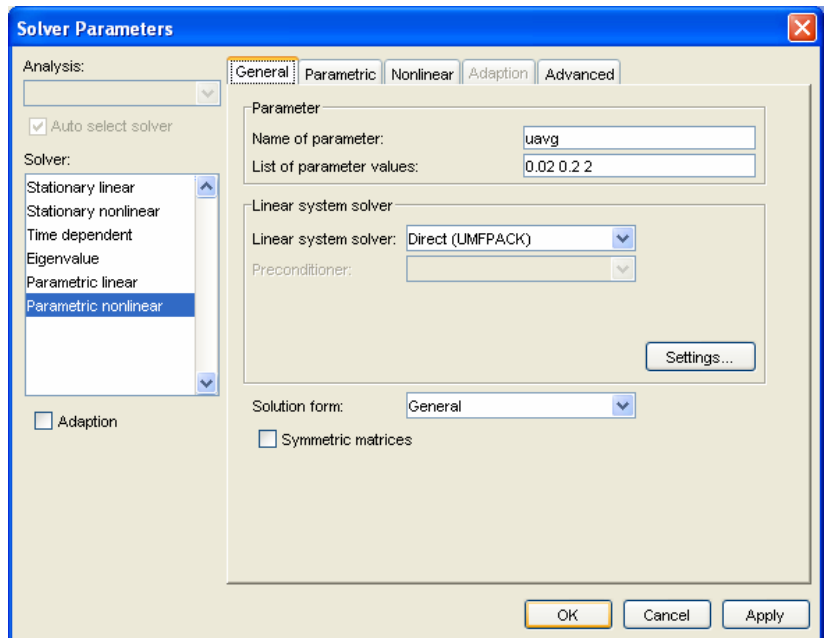
Now investigate the effect of changing the diffusivity and the average velocity of the fluid. In doing this you will examine the relative effect of diffusion and convection. The Peclet number gives the relative effect of these two quantities and is defined as

$$Pe = \frac{D_{AB}}{uD_t} = \frac{\text{Diffusion}}{\text{Convection}} \quad (7)$$

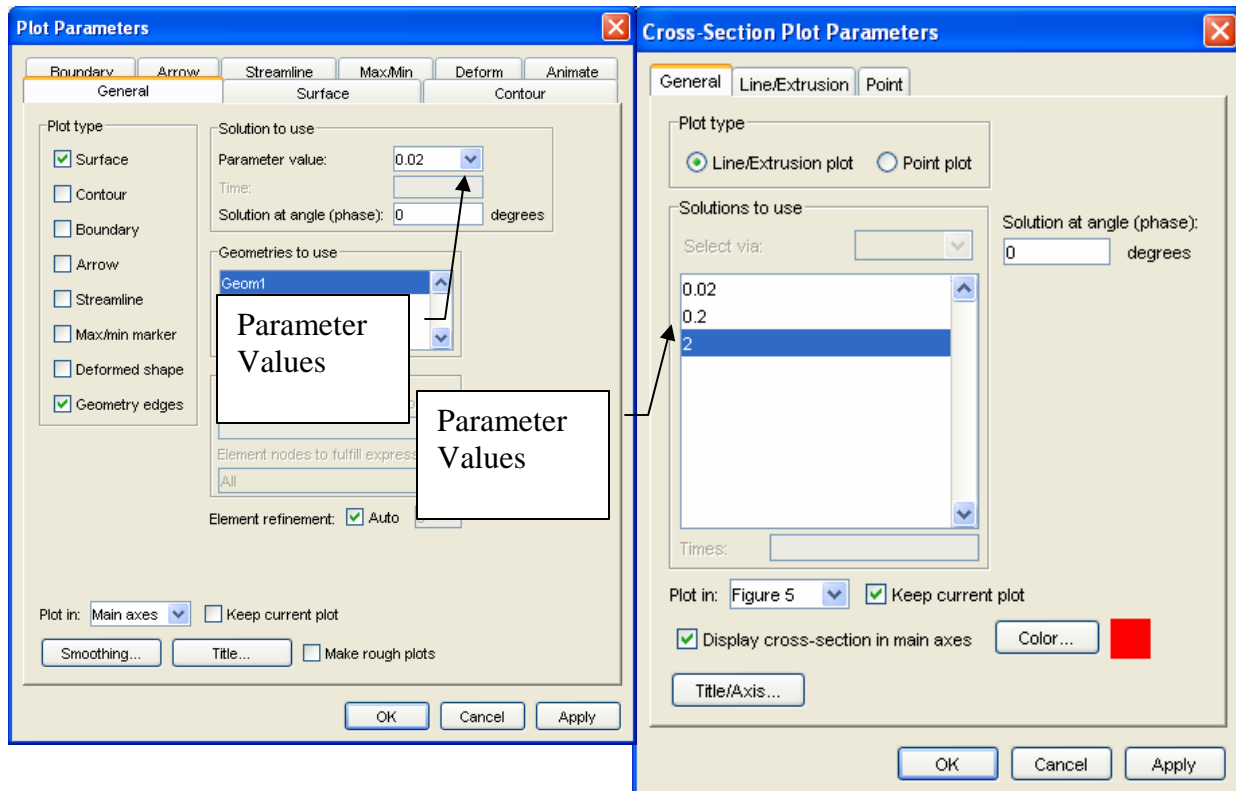
$u$ (m/s)	$D_{AB}$ (m <sup>2</sup> /s)	Re	$Pe = D_{AB}/(uD_t)$	Comments
0.02	2.69E-04	7.623	0.530	
0.2	2.69E-04	76.230	0.053	
2	2.69E-04	762.305	0.005	
0.02	2.69E-05	7.623	0.053	
0.02	2.69E-06	7.623	0.005	

To investigate the effect of changing the average velocity and diffusivity you should use the parametric solver. For the runs of varying velocity and

1. Choose the parametric solver by selecting **Solver > Parametric Solver**
2. Then give the parameter name and the values.



In making the plots you will need to choose the parameter value in the Solutions to use box.



**Submit:**

1. Plots Surface Plots Concentration and Cross-section plots (radial cross section with 5 z values) of concentration for.
  - 1.1. Plug Flow
  - 1.2. Laminar flow – no diffusion
  - 1.3. Laminar flow
    - 1.3.1. 3 diffusivities
    - 1.3.2. 2 velocities
2. Make a cross section plot with results from all 3 diffusivities on one plot. Write a comment on the effect of changing the diffusivity.
3. Make a comment on what has happened when the velocity changes from a low value to a high value.
4. Explain what Taylor dispersion is. You should refer to your Fogler text page 878 Section 14.2.2 (3<sup>rd</sup> edition)