Objectives:

- 1) Describe to a graduate student the difference between the prediction of the outlet conversion obtained from a model assuming plug flow and a laminar flow reactor model that contains both radial and axial diffusion.
- 2) This tutorial will have you compare the results of a POLYMATH plug flow reactor model with three models produced by COMSOL and solved using a finite element numerical method. The three models will be:
 - a) Plug flow reactor in laminar flow
 - b) Laminar flow reactor with axial diffusion
 - c) Laminar flow reactor with axial and radial diffusion

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

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

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

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

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

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

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

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

$$u_{z}\frac{\partial C_{A}}{\partial z} = D_{AB}\frac{\partial^{2}C_{A}}{\partial z^{2}} + D_{AB}\frac{\partial}{r\partial r}\left(r\frac{\partial C_{A}}{\partial r}\right) + r_{A}$$
(5)

Notice that if the diffusive flux in equation 5 is neglected ($D_{AB} = 0$) then the familiar plug flow reactor equation results

$$u_z \frac{\partial C_A}{\partial z} = r_A \tag{6}$$

The reaction stoichiometry is given by

$$A + B \Leftrightarrow 2C \tag{7}$$

The reaction rate is given by

$$r_{A} = -A \exp\left(-\frac{E}{RT}\right) \rho_{cat} \left(C_{A}C_{B} - \frac{C_{c}^{2}}{K_{eq}}\right)$$
(8)

In COMSOL the equation is written as:

$$rA = -A * \exp(-E/RT) * rhoCat * (cA * cB - cC^2/Keq)$$
(9)

For the isothermal reactor the T is set equal to T0.

The equilibrium constant is given by

$$K_{eq} = 1000 \exp\left(\frac{\Delta H_{Rx}}{R} \left(\frac{1}{303K} - \frac{1}{T}\right)\right)$$
(10)

Construct a polymath model for this problem given that the activation energy *E* is 95,238 J/mol, the preexponential is $A=1.1\times10^8$ m⁶/(mol kg s), and the heat of reaction is

 $\Delta H_{Rx} = -83680 J/mol$. The fluid is fed at an inlet temperature is 320K the inlet flowrate is

 5×10^{-4} m³/s. The reactant concentrations for A and B are equimolar at 500 mol/m³. The density of the catalyst is 1500 kg/m³. The reactor is 1 m in length with a radius of Ra=0.1 m.

To save time you can copy and paste the model given below. Make sure there are no mistakes in this model.

```
d(FA)/d(V) = rA \# molA/m^3
rA = -k * 1500 * (cA * cB - cC ^ 2 / Keq) # molA/m^3/s
d(FC)/d(V) = -2 * rA
FC(0) = 0
d(FB)/d(V) = rA
FB(0) = .25
FA(0) = 0.25
cA = FA / flow
cB = FB / flow
cC = FC / flow
delH = -83680
Keq = 1000 * exp(delH / 8.314 * (1 / 303 - 1 / T))
L = V / (pi * 0.1 ^ 2)
pi = 3.14159265359
k = 1.1e8 * exp(-95238 / 8.314 / T)
T0 = 320
flow = 5e-4 \# m^3/s
FT = FA + FB + FC
T = T0
FT0 = 0.5
X = (0.25 - FA) / 0.25
V(0) = 0
V(f) = 0.03141
```

- 1) Calculate the Reynolds number of this flow if the average density is 1000 kg/m^3 and viscosity is 0.0016 kg/(m s).
- 2) Submit a POLYMATH model of this process. Plot the molar flowrates and the conversion of A as a function of volume of reactor and length of reactor. (remember constants in POLYMATH are given using the ! function).

Since we are in laminar flow the parabolic velocity profile for a pipe flow is given as

$$u_z = 2 * u_0 \left(1 - \left(\frac{r}{R_a} \right)^2 \right)$$
(11)

With the average velocity or superficial velocity given by

$$u_0 = \frac{5 \times 10^{-4} \, m^3 / s}{\pi R_a^2} \tag{12}$$

The manual explaining today's tutorial is located on the webct.rowan.edu page under the heading **3.1 FEMLAB ECRE Manual. This manual is also on the CD that came with you textbook.** I have attached the appropriate pages from the manual that you need to skim in several pages following this one. You will be entering this model in the REAL version of COMSOL and must turn in all assignments using the COMSOL model. You are of course welcome to compare your answers with the prepackaged models on your CD FEMLAB3 ECRE-VERSION that came with the book.

1. Quickly review the model description on the following pages and make a sketch of the geometry and the boundary conditions for this geometry.

FEMLAB[®]

FEMLAB ECRE

VERSION 3.1

Model Description, Equations, and Input Data

This chapter uses the FEMLAB ECRE Version to study an elementary, exothermic, 2nd-order reversible reaction

 $A + B \Leftrightarrow 2C$

in a tubular reactor (liquid phase, laminar flow regime). To keep its temperature down, the reactor uses a cooling jacket with a variable coolant temperature. The following model setup proceeds in stages, gradually leading to the final configuration. The first version of the model deals with an isothermal tubular reactor with composition variations in both the radial and axial directions. The second stage extends the model to include the energy balance for the reactor. By this addition, the isothermal reactor is turned into an adiabatic reactor. The third stage introduces an isothermal cooling jacket, and finally the fourth stage models a non-isothermal cooling jacket.

The following section provides a general description for all of the above-mentioned models.

Model Description



Figure 2-1: Model geometry for the 2-dimensional rotationally symmetric models.

Figure 2-1 illustrates the model geometry. We assume that the variations in angular direction around the central axis are negligible, and therefore the model can be axi-symmetric.

The system is described by a set of differential equations on a 2D surface that represents a cross section of the tubular reactor in the z-r plane. That 2D surface's borders represent the inlet, the outlet, the reactor wall, and the center line. Assuming that the diffusivity for the three species is of the same magnitude, you can model the reactor using three differential equations; one mass balance for one of the species (as noted in the next section, mass balances are not necessary for the other two species), one heat balance for the reactor core, and one heat balance for the heating jacket. Due to rotational symmetry, the software need only solve these equations for half of the domain shown in Figure 2-1.

Model Equations

You describe the mass balances and heat balances in the reactors with partial differential equations (PDEs), while one ordinary differential equation (ODE) is required for the heat balance in the cooling jacket. The equations are defined as follows.

MASS BALANCE, SPECIES A:

$$D_p \frac{1}{r} \frac{\partial C_A}{\partial r} + D_p \frac{\partial^2 C_A}{\partial r^2} + D_p \frac{\partial^2 C_A}{\partial z^2} - 2U \left(1 - \left(\frac{r}{R}\right)^2\right) \frac{\partial C_A}{\partial z} + r_A = 0$$

where D_p denotes the diffusion coefficient, C_A is the concentration of species A, U is the flow velocity, R gives the radius of the reactor, and r_A is the reaction rate. In this model we assume that the species A, B, and C have the same diffusivity, which implies that we must solve only one material balance; we know the other species' concentrations through stoichiometry.

BOUNDARY CONDITIONS FOR THE MASS BALANCE:

• Inlet (z = 0)

$$C_A(r,0) = C_{A0}$$

• At the wall (r = R)

$$\frac{\partial C_A}{\partial r}(R,z) = 0$$

• Center (symmetry) line

$$\frac{\partial C_A}{\partial r}(0,z) = 0$$

The boundary condition selected for the outlet does not set any restrictions except that convection dominates transport out of the reactor. Thus this condition keeps the outlet boundary open and does not set any restrictions on the concentration.

• Outlet (z = L)

$$\frac{\partial C_A}{\partial z}(r,L) = 0$$

where L denotes the length of the reactor.

ENERGY BALANCE INSIDE THE REACTOR: 9

$$k\frac{1}{r}\frac{\partial T}{\partial r} + k\frac{\partial^{2}T}{\partial r^{2}} + k\frac{\partial^{2}T}{\partial z^{2}} - 2U\left(1 - \left(\frac{r}{R}\right)^{2}\right)\rho C_{p}\frac{\partial T}{\partial z} - r_{A}(-\Delta H_{Rx}) = 0$$

where k denotes the thermal conductivity, T is temperature, ρ is density, C_p equals the heat capacity, and ΔH_{Rx} is the reaction enthalpy.

BOUNDARY CONDITIONS FOR THE ENERGY BALANCE:

ი

• Inlet (z = 0)

$$T(r,0) = T_0$$

• At the wall (r = R)

$$-\frac{\partial T}{\partial r}(R,z) = \frac{U_k}{k}(T-T_a)$$

where T_a denotes the temperature in the cooling jacket.

• Center (symmetry) line

$$-\frac{\partial T}{\partial r}(0,z) = 0$$

As for the mass balance, choose the boundary condition at the outlet for the energy balance such that it keeps the outlet boundary open. This condition sets only one restriction, that the heat transport out of the reactor be convective.

• Outlet (z = L)

$$-\frac{\partial T}{\partial z}(r,L) = 0$$

ENERGY BALANCE OF THE COOLANT IN THE COOLING JACKET:

Here we assume that only axial temperature variations are present in the cooling jacket. This assumption gives a single ODE for the heat balance:

$$\frac{\partial T_a}{\partial z} = \frac{2\pi R U_k (T-T_a)}{m_c C_{Pc}}$$

where m_c is the mass flow rate of the coolant, C_{Pc} represents its heat capacity, and U_k gives the heat-transfer coefficient between the reactor and the cooling jacket. You can neglect the contribution of heat conduction in the cooling jacket and thus assume that heat transport takes place only through convection.

BOUNDARY CONDITION FOR THE COOLING JACKET:

You can describe the cooling jacket with a 1D line. Therefore you need only an inlet boundary condition.

• Inlet (z = 0)

$$T_a(0) = T_{a0}$$

Model Parameters

We now list the model's input data. You define them either as constants or as logical expressions in FEMLAB's **Option** menu. In defining each parameter in FEMLAB, for the constant's **Name** use the left-hand side of the equality in the following list (in the first entry, for example, Diff), and use the value on the right-hand side of the equality (for instance, 1E-9) for the **Expression** that defines it.

The constants in the model are:

- Diffusivity of all species, $Diff = 1E 9 m^2/s$
- Activation energy, E = 95238 J/mol

- Rate constant, $A = 1.1E8 \text{ m}^6/(\text{mol}\cdot\text{kg}\cdot\text{s})$
- Gas constant, R = 8.314 J/mol·K (do not confuse this constant with the geometrical extension of the radius)
- Inlet temperature, T0 = 320 K
- Total flow rate, $v0 = 5 \text{ E}-4 \text{ m}^3/\text{s}$
- Reactant concentrations in the feed, $CAO = CBO = 500 \text{ mol/m}^3$
- Reactor radius, Ra = 0.1 m
- Catalyst density, ρ_{Cat} , rhoCat = 1500 kg/m³
- Heat of reaction, ΔH_{Rx2} dHrx = -83680 J/mol
- Equilibrium constant at 303 degrees K, Keq0 = 1000
- Thermal conductivity of the reaction mixture, $ke = 0.559 \text{ J/m} \cdot \text{s} \cdot \text{K}$
- Average density of the reaction mixture, ρ , rho = 1000 kg/m³
- Heat capacity of the reaction mixture, $Cp = 4180 \text{ J/kg} \cdot \text{K}$
- Overall heat-transfer coefficient, $Uk = 1300 \text{ J/m}^2 \cdot \text{s} \cdot \text{K}$
- Inlet temperature of the coolant, Ta0 = 298 K
- Heat capacity of the coolant, $CpJ = 4180 \text{ J/kg} \cdot \text{K}$
- Coolant flow rate, mJ = 0.01 kg/s

Next, the following section lists the definitions for the expressions this model uses. Again, to put each expression in FEMLAB form, use the left-hand side of the equality (for instance, u0) for the variable's **Name**, and use the right-hand side of the equality (for instance, v0/($pi*Ra^2$)) for its **Expression**.

• The superficial flow rate is defined according to the analytical expression

$$u_0 = \frac{v_0}{\pi (Ra)^2}$$

which we define in FEMLAB as $u0 = v0/(pi*Ra^2)$.

• The superficial, laminar flow rate

$$u_z = 2u_0 \left(1 - \left(\frac{r}{Ra}\right)^2\right)$$

in FEMLAB form becomes $uz = 2*u0*(1-(r/Ra).^2)$.

• The conversion of species A is given by

$$x_A = \frac{C_{A0} - C_A}{C_{A0}}$$

which in FEMLAB form is xA = (cA0 - cA) / cA0.

• The concentration of B is according to

$$C_B = C_{B0} - C_{A0} x_A$$

which in FEMLAB form becomes cB = cB0-cA0*xA.

• The concentration of C is expressed as

$$C_c = 2C_{A0}x_A$$

which in FEMLAB form becomes cC = 2*cA0*xA.

- The rate of reaction takes two forms:
 - Before adding the heat balance, the reaction looks like

$$r_A = -A \exp\left(-\frac{E}{RT_0}\right) \rho_{cat}\left(c_A c_B - \frac{c_c^2}{K_{eq}}\right),$$

which in FEMLAB form is $rA = -A*exp(-E/R/T0)*rhoCat*(cA*cB-cC^2/Keq)$.

- After you add the energy balance, the reaction expression becomes

$$r_A = -A \exp\left(-\frac{E}{RT}\right) \rho_{cat}\left(c_A c_B - \frac{c_c^2}{K_{eq}}\right),$$

which in FEMLAB form is $rA = -A*exp(-E/R/T)*rhoCat*(cA.*cB-cC^2/Keq)$.

- The temperature-dependent equilibrium constant is given by the following expressions:
 - For the isothermal case

$$K_{eq} = K_{eq0} \exp\left(\frac{\Delta H_{Rx}}{R}\left(\frac{1}{303} - \frac{1}{T_0}\right)\right)$$

which in FEMLAB form is Keq = Keq0*exp(dHrx/R*(1/303-1/T0)).

- After adding the energy balance you obtain

$$K_{eq} = K_{eq0} \exp\left(\frac{\Delta H_{Rx}}{R}\left(\frac{1}{303} - \frac{1}{T}\right)\right)$$

which in FEMLAB form is Keq = Keq0 * exp(dHrx/R*(1/303-1/T)).

• The heat-production term becomes

$$Q = -r_a \Delta H_{Rx}$$

which in FEMLAB form is Q = -rA*dHrx.

- 2. Open Comsol Multiphysics 3.4, Select the New Tab, Choose Axial symmetry (2D).
- 3. Choose Chemical Engineering Module, Mass balance, Convection and Diffusion, Steadystate analysis.
- 4. In the Dependent variables space replace the c with cA

Model Navigator	
Multiphysics Component Library User Components	Choose Axial symmetry (2D) from the drop down menu
Space dimension: Axial symmetry (2D)	Multiphysics
Application Modes COMSOL Multiphysics Chemical Engineering Module Chemical Engineering Module Chemi	Add Remove Add Remove Geom1 (2D) Select Convection & Diffusion, Steady-state analysis on Independent variables: r phi z Application Mode Properties Add Geometry Add Frame Ruling application mode:
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- 5. Select Add
- 6. Select OK
- 7. Now you must draw the geometry of a tube in COMSOL. This is a rectangle. Remember that the center of the pipe is at a radial position of 0 and the wall of the pipe is at a dimension of 0.1m. The length of pipe will be set at 1m.

- 8. For this model the length of the reactor is much longer than radius. To see the trends in both directions a set of unequal axes can be obtained. To obtain an "unequal" axes setting, Choose Options, Axis/Grid settings and select the Axis tab and then clear the Axis equal check box. Enter -0.1 in the r min edit field, 0.2 in the r max edit field and -0.1 and 1.1 in the z min and z max edit fields, respectively. To obtain a Grid spacing of 0.1 go to the Grid tab and click on the Auto box. Change the settings to 0.1 and 0.1. Then Click OK
- 9. Now draw the rectangle that represents half of a reactor. (eg. from r=0 to r=0.1m and z=0 to z=1.0m.
- 10. Go to the Physics menu and select Subdomain Settings, which opens up the corresponding dialog box. Select subdomain 1 in the Subdomain Settings list. This dialog box displays the equation that forms the basis for

Subdomain S

this application mode, while the edit fields show the input data used in the equation.

- 11. Now choose Physics, subdomain Settings and select subdomain 1. Enter Diff, rA, 0 and uz as shown in the figure below. The edit fields correspond to the diffusion coefficient, reaction-rate expression, and velocity distribution in the reactor—all of which you can freely define. To review and change the definition of the input data, follow this procedure
- 12. Select the Init tab (this sets the initial conditions for the reactor) Now enter cA0 in the initial value box.

Axes/Grid	Settings 🛛 🔀
Axis Grid	
Axis e r-z limits r min: r max: 0 z min: z max: 1	qual 0.1 I.2 0.1 phi min: phi max: 500
	OK Cancel Apply
Rectan	gle 🔰
Size Width: Height:	0.1 a: 0 (degrees) 1 1 1 1
Position	
Base: r: z:	Corner Style: Solid 0 Name: R1
C	OK Cancel Apply Help
ings - Cor	vection and Diffusion (chcd)

Subdomains Groups	C Init Element C	plor		
Subdomain selection	Species			
1	Library material:	~	Load	
	Quantity	Value/Expression	Unit	Description
	δ _{ts}	1		Time-scaling coefficient
	💿 D isotropic	Diff	m²/s	Diffusion coefficient
	🔿 D anisotropic	1001	m²/s	Diffusion coefficient
✓	R	rA	mol/(m ³ ·s)	Reaction rate
Group:	u	0	m/s	r-velocity
Select by group	v	uz	m/s	z-velocity
C Active in this domain	Artificial Diffusio	pn		

Subdomain Settings - Convection and Diffusion (chcd)

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$\delta_{ts} \partial c / \partial t + \nabla (- \nabla \nabla c) = R - \mathbf{u}$	∇c , c = concentration	
Subdomains Groups	c Init Element Color	
Subdomain selection	Initial value	
1	Variable Initial value	Unit Description
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🌀 Constan	ts			
Name	Expression	Value	Description	
Diff	1e-9	1e-9		~
E	95238	95238		
A	1.1e8	1.1e8		
R	8.314	8.314		
ТО	320	320		
v0	0.0005	5e-4		
cA0	500	500		
cB0	500	500		
Ra	0.1	0.1		
rhoCat	1500	1500		
dHrx	-83680	-83680		
Keq0	1000	1000		
				~
i 🛱		OK Cance	el Apply H	Help

13. Select Options, Constants and then enter Constants -

14. Select Options, Scalar Expressions and enter the following expressions. Some of these expressions

will be used in later models.

🐨 Scalar	Expressions	×
Name	Expression Description	
uO	v0/(pi*Ra^2)	~
uz	2*u0*(1-(r/Ra)^2)	
хA	(cA0-cA)/cA0	
сB	cB0-cA0*xA	
cC	2*cA0*xA	
rA	-A*exp(-E/R/T0)*rhoCat*(cA*cB-cC^2/Keq)	
Keq	Keq0*exp(dHrx/R*(1/303-1/T0))	
		~
i 🖉 🖬	OK Cancel Apply Help	

15. Go to the **Physics** menu and select **Subdomain Settings**, which opens up the corresponding dialog box. Select subdomain 1 in the Subdomain Settings list. Enter the reaction rate rA, the z-velocity and the diffusion coefficient Diff

$\delta_{ts}\partial cA/\partial t + \nabla \cdot (-D \nabla cA + cA$	Au) = R, cA = concentration
Subdomains Groups	CA Init Element Color
Subdomain selection	Species
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	Quantity Value/Expression Description
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	R rA Reaction rate
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🗹 Active in this domain	Artificial Diffusion
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to the Init tab and	OK Cancel Apply Help enter the initial concentration variable cA0 and then se
o to the Init tab and ubdomain Settings - Co	OK Cancel Apply Help enter the initial concentration variable cA0 and then se onvection and Diffusion (MassBalance)
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OK

Cancel

Apply

Help



will flow out of the reactor at boundary 3.

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	N ₀	0	Inward flux	L			N ₀	0	Inward flux
Select by group				L	Select by group				
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OK Cancel Apply OK Cancel Apply									
10		~ .					-		

- 18. Now create a mesh. Go to the Mesh mode by pressing the mesh mode button.
- 19. Select Mesh, Initialize Mesh. This will automatically create a mesh for you.





- 20. You should probably refine this mesh by choosing the Mesh, Refine Mesh option. Notice the short cut figure for later refining of the mesh. To obtain the images that are shown later you will need to refine certain areas of the mesh. This can be done by choosing the Mesh, Refine Selection button or option.
- 21. Note in this case that the scales on the r- and z-axes are not equal, which gives a distorted view. If desired, you can select equal scale settings in the Axis/Grid Settings menu item under the Options menu. In order to return to the original unequal scale settings, once again go to the Axes/Grid Settings menu and clear the Axis equal check box. Enter -0.1 in the r min edit field, 0.2 in the r max edit field and -0.1 and 1.1 in the z min and z max edit fields, respectively.
- 22. The model in this exercise is nonlinear; thus press the Solver Parameters and verify that the Stationary nonlinear solver is selected.
- 23. Solve the problem using the Solve Problem button or drop down menu.

Solver Parameters		X
Analysis:	General Stationary Adaptive Advanced	
Stationary Auto select solver Solver: Stationary Time dependent Eigenvalue Parametric Stationary segregated	Linear system solver Linear system solver: Direct (UMFPACK)	
Parametric segregated	Matrix symmetry: Nonsymmetric	
	OK Cancel Apply Help	





I Click the **Postprocessing Mode** button. The default plot shows the concentration of species A in the reactor.



2 Click the **Plot Parameters** button.



3 Click on the **Surface** tab.

4 On the **Surface** page, enter - rA in the **Expression** edit field.

🗹 Surface plot	
Surface data	
Predefined quantities:	Range
Expression:	-rA Smooth
Height data	
Predefined quantities:	Concentration, cA
Expression	cA
Coloring: Interpo	lated V Fill style: Filled V
 Colormap: Uniform color: 	jet Colors: 1024 Color scale Color

5 Click Apply.



6 To plot the conversion of species A, enter xA in the Expression edit field in the Plot Parameters dialog box.



7 Click Apply.

- 8 In order to define the location of the maximum and minimum conversion, click the Max/Min tab.
- 9 Enter xA in the Expression edit field in the Subdomain max/min data dialog box.
- **IO** Click the **Max/min marker** check box and click **Apply**.
- II To visualize the relation between residence time and conversion, first click the Max/ min marker check box to deselect it and click the Arrow tab in the Postprocessing menu.
- 12 Select Total flux, cA in the Predefined quantities drop-down list.





- **I4** To visualize the local conversion in selected cross sections along the length of the reactor, first go to the **Postprocessing** menu and select **Cross-Section Plot Parameters**.
- **I5** Click the Line/Extrusion tab.
- **I6** Enter xA in the **Expression** edit field.
- **I7** Enter 0 in the **r0** edit field and 0.1 in the **r1** edit field.
- **I8** Enter **0** in both the **z0** and **z1** edit fields.
- 19 Check the Multi parallel lines box, then click the Vector with distances option.

20 Enter 0 0.5 1 in the **Vector with distances** edit field to generate three cross-section plots at the inlet, in the middle of the reactor, and at the outlet, respectively.

oss-Section Plot Para	neters		
General Line/Extrusion p	oint		
 Line/Extrusion plot 			
Plot type			
💿 Line plot	O Extrusion p	lot	
y-axis data			
Predefined quantities:			*
Expression:	۱		
x-axis data	Cross-section	line c	lata
Arc-length	r0: 0	r1:	0.1
O Expression	z0: 0	z1:	0
	Line resolution	C.	200
- 🗹 Multiple parallel lines -			
Number of lines	Vector wit	h dist	ances
	00.51		
Line Settings	Surface Setting	s.,,.	
	OK Car	cel	Apply

21 Click the **Line Settings** button. In the dialog box that opens, select the **Cycle** option in the **Line color** drop-down list; select **Dotted line** in the **Line style** drop-down list; and select **Cycle** in the **Line marker** drop-down list.

Line color:	Cycle	~	Color	
Line style:	Dotted line	~		
Line marker:	Cycle	~		
Legend				

See note on making graphs on page 27 of 31 of this pdf file step 15 and then return

2 Finally, to generate the following plot, click **OK** twice: first in the **Line Settings** dialog box, and then in the **Cross-Section Plot Parameters** dialog box.

Radial Conversion Profiles



Figure 2-2: Radial conversion profiles at the inlet, outlet and halfway through an isothermal reactor.

24. In Step 22 of the pdf file it asked you to make a Cross-Section plot. I prefer to use as the x-axis data the r coordinate. Also in the line Settings box I always request a legend.



- 25. Also a title to the graph as well as axis labels can be specified. Select the General tap and the Title/Axis button.
- 26. This plot can now be pasted into a word document by selecting the MS windows copy icon.

Title/Axis Settings Image: Cross Section Plot of the Isothermal Laminar Flow r Title: Auto Cross Section Plot of the Isothermal Laminar Flow r Axis settings for line and point plots First axis label: Auto Radius (m) Log scale Second axis label: Auto Conversion of A Log scale OK Cancel



Cros	s-Section Plot Parameters	
Ger	neral Line/Extrusion Point	
0	Line/Extrusion plot	
ГР	lot type	
(Line plot O Extrusion plot	
ſ	-axis data	
P	redefined quantities:	
E	xpression: XA	
	• r • • r • • Expression • • Line resolution: 200	
Ē	Multiple parallel lines	
	Line Settings OK Cancel Apply	
	Cross-Section Plot Parameters	×
	General Line/Extrusion Point	
	Plot type	
	O Line/Extrusion plot ○ Point plot	
	Solutions to use Solution at angle (phas	e):
- 1 - 2	Select via: O degree	s
- 3	Title/Axis Button	
	Times:	
	Plot in: Figure 1 📉 🗌 Keep current plot	
	Display cross section in main axes Color	
	Title/Axis	



- 27. To obtain a table of data shown on the cross section plot then you must click on the ASCII button and then save this file.
- 28. The file will be a text file that can be opened by excel for further analysis. Open the txt file by having excel look for text files.
- 29. Then start the conversion of the data using a delimited file.∖

Text Import Wizard - Step 1 of 3			? 🗙		
The Text Wizard has determined that you If this is correct, choose Next, or choose	ır data is Delimited. the data type that be	st describes your data.			
Original data type Choose the file type that best describes your data: Delimited - Characters such as commas or tabs separate each field. - Fixed width - Fields are aligned in columns with spaces between each field. 					
Start import at <u>r</u> ow: 1	🗘 File <u>o</u> rigin:	437 : OEM United States	~		
Preview of file C:\Documents and Settin	gs\H\cross-sectiond	lata isothermal laminar.txt.			
1 * Coordinates					
3 5.02512568-4	0.0 -1.1368684 E -16				
40.0010050251	0.0				
<u>5</u> 0.0015075378	0.0		~		
			>		
(Cancel < Ba	ack <u>N</u> ext > <u>F</u> ir	iish		



Text Import Wizard - Step 2 of 3	?	×
This screen lets you set the delimiters your data contains. You can see how your text is affected in the preview below.		
Delimiters		
I Iab Semicolon Comma		
✓ Space Other: Text gualifier:		
Data preview		h
* Coordinates	^	J
p.o p.o		
5.0251256E-4 -1.1368684E-16		
	_	
0.0015075578 0.0	~	
Cancel <u>Back</u> <u>Next</u> <u>Finis</u>	h	J

30. The data is placed in two columns (x,y). The first cross-section at z=0m is listed, followed by the second cross-section z=0.5m, followed by the third cross-section at z=1.0m. To find these I always use the Edit, Search feature and find the ending r data point.

N	licrosoft Ex	cel - cros	s-sectiond	ata isothe	rmal la	amina	X I	Aic rosoft	Excel - cros	ss-section	data isoth	ermal laı
:2)	<u>File E</u> dit	<u>V</u> iew <u>I</u> ns	ert F <u>o</u> rmat	<u>T</u> ools	<u>D</u> ata	<u>W</u> indov	:2	<u>F</u> ile <u>E</u> dit	<u>V</u> iew <u>I</u> n	sert F <u>o</u> rm	at <u>T</u> ools	<u>D</u> ata <u>W</u>
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199	0.098995	0					199	0.09899	5 C)		
200	0.099497	0					200	0.099493	7 0)		
201	0.1	0	End of dat	a for z=Om	n		201	0.1	I C	End of d	<u>ata</u> for z=0i	n
202	0	0.269076	Start of da	ia for z=0.	.5m		202	1	0.269076	Start of o	la <mark>i</mark> a for z=C).5m
203	5.03E-04	0.269081					203	5.03E-04	1 0.269081			
204	0.001005	0.269096					204	0.00100	5 0.269098	i		
205	0.001508	0.269121					205	0.00150	3 0.269121			
206	0.00201	0.269155					206	0.0020	I 0.269155	5		
400	0.099497	0.950558					598	0.098492	2 0.957453	}		
401	0.1	0.960809	End of dat	a for z=0.5	5		599	0.09899	5 0.964472	2		
402	0	0.424049	Start of da	ta for z=1.	.0m		600	0.099497	0.969844	1		
403	5.03E-04	0.424055					601	0.1	0.973568	B End of d	ata for z=1.	Om
404	0.001005	0.424074					602	%	Elements	(triangula	ar)	
405	0.001508	0.424105					603		1 2	2		
406	0.00201	0.424148					604		2 3	}		
407	0.002513	0.424203					605		3 4	1		
408	0.003015	0.424271					606		1 E	5		
409	0.003518	0.424352					607		5 6	ì		
410	0.00402	0.424444					608	(6 7	7 		
411	0.004523	0.424549					609		7 8	}		
412	0.005025	0.424667					610	1	3 9	9		
413	0.005528	0.424797					611		3 10)		
414	0.00603	0.424939					612	11] 11			
415	0.006533	0.425094					613	1	12	2		
416	0.007035	0.425261					614	1.	2 13	}		
417	0.007538	0.425441					615	1.	5 14	•		_
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Find	Replace	
Fi <u>n</u> d what	t: 0.1	~
	[Op <u>t</u> ions >>
	Find All Eind Next	Close

FEMLAB ECRE can also calculate integral expressions of the solution. One such entity is the mixing cup outlet concentration, which gives the average concentration in the liquid that exits the reactor. For species A, the average concentration is defined according to the equation

$$C_{A, av} = rac{\int 2\pi r C_A u_z dr}{\int 2\pi r u_z dr}$$

along the outlet boundary. Start by calculating the integral of $C_A u_z$ over the outlet boundary.

2 Go to the **Postprocessing** menu and select **Boundary Integration**.

24 Select boundary 3 in the Boundary selection list.

25 Enter 2*pi*r*cA*uz in the Expression edit field.

26 Click Apply.

The value of the integral appears in the status bar at the bottom and reads 0.114385. You can now calculate the integral of u_z .

27 Enter 2*pi*r*uz in the Expression edit field and click Apply.

The value of this integral is 5e-4, which gives an average concentration of 0.114385/5e-4, which is approximately 230 mole m⁻³.

You have now completed a review of the model and are ready to run it with varying input parameters.

Questions and Exercises

To answer the following questions you can either use the results in the model just described or you can solve it again with a new set of input data.

- I Why is the concentration of species A near the reactor wall lower than the concentration near the center?
- 2 Where in the reactor do you find the minimum and maximum reaction rates?
- **3** How much is the average conversion? (Hint: See the calculation of the average concentration in the previous section.)
- **4** This exercise requires that you change the activation energy for the reaction in the model. Do so by going to the **Options** menu and working with the **Constants** menu item (see item 5 in the section "Model Equations and Input Data" on page 21). We have already tabulated the notations in the section "Model Parameters" on page 15. After changing the input data, click the **Solve** button to solve the problem.



It is useful to take the graphs you obtain by changing the activation energy and examine them in both two and three dimensions. Once in the Postprocessing mode you can toggle between a two- and three-dimensional plot by clicking the **2D Surface Plot** button or **3D Surface Plot** button.



- **a** How do the conversion profiles and the average conversion change if you increase the activation energy by a factor of 1.5?
- **b** How do these same entities change if you decrease the activation energy by multiplying the original value by a factor of 0.95?

The reaction rate is very sensitive to changes in activation energy. Altering the activation energy to a lower value increases the reaction rate. A high reaction rate in combination with the low flow rate close to the wall results in very large concentration gradients. In order to capture an accurate concentration profile, you must apply a dens mesh in the inlet area near the wall.

You have now investigated the isothermal reactor example. Let's proceed by introducing the energy balance in the reactor.

To be Submitted:

- 1) POLYMATH model and requested plots
- 2) Reynolds number calculations
- 3) Answer Questions 1-4 on pages 29 and 30 of 32 in the pdf file (ECRE tutorial pages 31&32).
- Reset your model to the base case conditions. Now run the COMSOL model with the diffusivity set to zero and remove the parabolic velocity profile by setting the z-velocity to the average velocity of u0.
 - a) Produce a surface plot and a crosssection plot to compare with the previous case of laminar flow.
 Compare the base case with the case of zero diffusivity and a uniform velocity profile.
 - b) Make a new cross section plot of conversion as a function of axial position. Choose to plot in a new figure and keep your old plot. You

Subdomain Settings - Convection and Diffusion (MassBalance) 🛛 🛛 🔀					
Equation ⊽•(-D⊽cA+cAu) = R, cA = cc	oncentration				
Subdomain selection	CA Init Element				
1	Species				
	Library material:	💌 🔽	pad		
	Quantity	Value/Expression	Description		
	ō _{ts}	1	Time-scaling coefficient		
	 D isotropic 	0	Diffusion coefficient		
	🔘 D anisotropic	1001	Diffusion coefficient		
	R	rA	Reaction rate		
~	u	0	r-velocity		
Select by group	v	uO	z-velocity		
Active in this domain	Artificial Diffusi	on			
OK Cancel Apply					

will need to change your titles. Make a plot in excel of this data compared to X_A vs L data obtained from your POLYMATH model.

- c) Compare the average outlet conversion from the COMSOL laminar flow model (base case) with the conversions obtained from the POLYMATH PFR model and the COMSOL model with zero diffusivity and the uniform velocity profile. Write a statement on the comparison of the conversion of these two data sets.
- 5) Reset the base case to have only axial diffusion with value of Diff=1e-2 m^2/s . See Figure on next page. Then repeat the analysis in steps a though c of question 4).

Cross-Section Plot Parameters	Cross-Section Plot Parameters
General Line/Extrusion Point Plot type Ine/Extrusion plot Plot type Solutions to use Select via: Image:	General Line/Extrusion Point Image: Description of the struston plot Image: Description of the struston plot Plot type Image: Description of the struston plot Image: Predefined quantities: Image: Description of the struston plot Image: Predefined quantities: Image: Description of the struston plot Image: Description of the struston plot plot plot plot plot plot plot plot
Plot in: Figure 2 ♥ ♥ Keep current plot ♥ Display cross-section in main axes Color Title/Axis OK Cancel Apply	Number of lines Vector with distances 5 0 0.05 0.1 Line Settings Surface Settings
	OK Cancel Apply

Subdomain Settings - Con	vection and Diffu	ision (MassBalanc	e)	×	
Equation ∇•(-D⊽cA+cAu) = R, cA = co	ncentration				
Subdomain selection	cA Init Element				
1 Species					
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		ок	Cancel Apply		

In the Table for anisotropic the Diffusivities are:

Dr (radial)	
	Dz (axial)