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 and conduction.
- 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 and radial diffusion and conduction

Adiabatic Reactor

This second model with radial effects adds a heat balance to the material balance in the previous model. We assume the reactor is adiabatic, which means that its walls are insulated and do not exchange heat with the surroundings. To generate this model you should start with your previous comsol model or use the model linked to webct. In this new model that you will generate you will add an additional application mode for energy balances to the mass balances already included in the previous model.

Mole Balances

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. 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 then the familiar plug flow reactor equation results

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

The steady-state energy balance on the fluid within the reactor can be transformed to the following equation (See Section 8.9 in Fogler 4th edition)

$$0 = -\frac{\partial}{\partial z} \left(-k \frac{\partial T}{\partial z} + C_p u_z T \right) - \frac{\partial}{r \partial r} \left(-k r \frac{\partial T}{\partial r} \right) + r_A \Delta H_{Rx}$$
(7)

The reaction stoichiometry is given by

$$A + B \Leftrightarrow 2C \tag{8}$$

The reaction rate is given by

$$r_{A} = -A \exp\left(-\frac{E}{RT}\right) \rho_{cat} \left(C_{A}C_{B} - \frac{C_{c}^{2}}{K_{eq}}\right)$$
(9)

In COMSOL the equation is written as:

$$rA = -A * \exp(-E/RT) * rhoCat * (cA * cB - cC^2/Keq)$$
⁽¹⁰⁾

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

The equilibrium constant is given by

$$K_{eq} = 1000 \exp\left(\frac{\Delta H_{Rx}}{R} \left(\frac{1}{303K} - \frac{1}{T}\right)\right)$$
(11)

Using your previous polymath model, add an energy balance of a PFR to this model.

$$\frac{\mathrm{d}T}{\mathrm{d}V} = \frac{Ua(T_a - T) + \Delta H_R|_T r_A}{\left(\sum_{i=1}^n F_{i0}C_{pi} + F_{A0}X\Delta C_p\right)}$$
(12)

Assume that the heat capacity of the reaction mixture is $Cp = 4180 \text{ J/kg} \cdot \text{K}$ (e.g. $\Delta C_p = 0$), the

thermal conductivity of the reaction mixture is $k = 0.559 \text{ J/m} \cdot \text{s} \cdot \text{K}$, and for the reactor with cooling the overall heat-transfer coefficient, Ua = 1300 J/m² \cdot \text{s} \cdot \text{K}. Your previous model has a reaction with an activation energy *E* is 95,238 J/mol, the pre-exponential is A=1.1×10⁸ m⁶/(mol kg s), and the heat of reaction is $\Delta H_{Rx} = -83680 \text{ J / mol}$. 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 and the liquid phase density is 1000 kg/m³. The reactor is 1 m in length with a radius of Ra=0.1 m. For the polymath model you will need the heat capacity with units of molar heat capacity which can be found as

$$C_{P(MOLAR)} = \frac{C_{P(MASS)}\rho v_0}{F_T}$$
(13)

Submit all work in email with the subject title, "Comsol Adiabatic Reactor." All "printouts" should be pasted into a word document and submitted by email. Answer any questions using text in the word document. Place figure captions on all figures to explain what you have plotted.

- 1) Submit your new POLYMATH model of this process (Paste the output into MS word document).
 - a) This first model will be of an adiabatic reactor
 - b) The second model will include an overall heat transfer term ($U_k = 1300 \text{ J/m}^2 \cdot s \cdot K$).
- 2) Plot the temperature and 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

$$u_z = 2 * u_0 \left(1 - \left(\frac{r}{R_a}\right)^2 \right)$$
(14)

With the average velocity or superficial velocity given by

$$u_0 = \frac{5 \times 10^{-4} \, m^3 / s}{\pi R_a^2} \tag{15}$$

- 1. Open Comsol Multiphysics and load your previous model. If this is not available load the file: 1-Isothermal_Reactor.fl from webCT.
- 2. Select Multiphysics, Model Navigator
- 3. Choose Chemical Engineering Module, Energy balance, Convection and Conduction.

Model Navigator	Select Convection &	z Conduction. Steady-state analysis
Space dimension:	Axial symmetry (2D)	Multiphysics
Application Modes COMSOL Multiph Comsol Engines Convect Convect Convect Conduct Conduct Mass balance Convect C	ysics ering Module nce ior and Conduction ady-state analysis issient analysis ion ady-state analysis ion and Diffusion ady-state analysis issient analysis Stefan Diffusion and Convection Planck Planck without Electroneutrality	Add Remove Geom1 (2D) Convection and Diffusion (chcd) Convection and Conduction (chcc) Convection a
Application mode name:	chcc2	Convection and D Select OK
Element:	Lagrange - Quadratic 🛛 👻	Multiphysics
		OK Cancel Help

- 4. Select OK
- 5. Remember that the geometry of the tube a rectangle. 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.

6. Enter the following Constants in **Options Constants** menu– Note some of these have already been added

Constants	i			×
Name	Expression	Value	Description	
Diff	1e-9	1e-9		
E	95238	95238		1
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		
ke	0.559	0.559	-	
rho	1000	1000		
Ср	4180	4180	· · · · · · · · · · · · · · · · · · ·	•
🖻 🔒		OK Canc	el Apply Help	

7. Enter in the **Options Expressions, Scalar Expressions** menu. **YOU MUST CHANGE YOUR TEMPERATURE VARIABLE IN THE REACTION RATE EXPRESSION.**

Scalar E	xpressions		×
Name	Expression	Description	
u0	v0/(pi*Ra^2)		~
uz	2*u0*(1-(r/Ra)^2)		
×A	(cA0-cA)/cA0		
сВ	cB0-cA0*xA		
cC	2*cA0*xA		
rA	-A*exp(-E/R/T)*rhoCat*(cA*cB-cC/Keq)		
Keq	Keq0*exp(dHrx/R*(1/303-1/T))		
Q	(-rA)*(-dHrx)		
			~
🖻 🖬	OK Cancel	Apply Help	

8. Select the **Physics** menu and select **Subdomain Settings** to open the corresponding dialog box. Select **subdomain 1** in the Subdomain selection list. This dialog box also displays the equation that forms the basis for the Conduction and Convection application mode, and the edit fields show the input data used in the energy balance. Note if you don't have a Time scaling coefficient that is ok.

Subdomain Settings - Cor	nvection and Condu	uction (EnergyBal	ance)	×			
Equation ∇∙(-k∇T + Σ _i h _i N _{D,i}) = Q - ρC _p u∙∇T, T= temperature							
Subdomain selection	Physics Init Elemen	t					
<u> </u>	Thermal properties a	nd heat sources/sinks					
	Library material:	🔽 🚺 Loa	id				
	Quantity	Value/Expression	Description				
	δ _{ts}	1	Time-scaling coefficient				
	💿 k (isotropic)	ke	Thermal conductivity				
	🔘 k (anisotropic)	400 0 0 400	Thermal conductivity				
	ρ	rho	Density				
	С _р	Ср	Heat capacity				
	Q	Q	Heat source				
	u	0	r-velocity				
	V	uz	z-velocity				
Select by group	n _i n _{D,i}	Species diffusion ina	active Species diffusion				
Active in this domain							
			OK Cancel Apply				

9. Here you are entering the variables that were given by equation 7. In the init tab for initial condition put T0.

Subdomain Settings - Convectio	n and Conduction (Energ	gyBalance)								
Equation ∇•(-k⊽T + Σ _j h _i N _{D,i}) = Q - ρC _p u∙⊽T, T= temperature										
Subdomain selection Physics Init Element										
	1 Initial value									
Vari	able Initial value	Description								
T(t ₀)	ТО	Temperature								
Select by group										
Active in this domain										
		OK Cancel	Apply							

10. Enter boundary conditions, axial symmetry for 1 and insulation for 4, Temperature, T0 for the inlet boundary 2 and convective flux for the reactor outlet 3. Notice when you click on the number the figure of the reactor highlights in red the boundary condition. Notice how the boundary is marked with a red line when you click in the Boundary Selection box.



11. To visualize the mesh click the Mesh Mode button. Note that the scales on the r- and z-axes are not



equal, which results in a distorted view. If desired, you can select equal scale settings by going to the **Options** menu and checking the **Axis** equal box in the **Axis/Grid Settings** menu item. 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.

12. The model we solve in this exercise is nonlinear. To verify the solver settings, click the Solver Parameters button and make certain that the Stationary nonlinear solver is selected.



Now Solve by pressing the "equal" sign

- 13. The manual explaining a portion of today's tutorial is located on the following pages and also on webct.rowan.edu page under the heading 3 Additional Materials, 3.1 FEMLAB ECRE Manual and is on CD with Book. This will open a pdf file titled FEMLAB3 ECRE version. 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.
- 14. You will now refer to the instructions in the ECRE manual which are given on the next page. This is written in the form of *look at what is in the ECRE model*. (This section was taken from page 39 step 1 of the manual which is 43 of 88 in the ECRE pdf file.)

GO to the next page

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 the **Surface** tab.

4 On the Surface page, go to the Predefined quantities drop-down list and select Temperature.



5 Click Apply.



6 To plot the conversion of A, enter xA in the **Expression** edit field in the **Surface** page.

7 Click Apply.



- **8** To visualize the relation between temperature and conversion, first click the **Contour** tab.
- **9** Select Temperature (EnergyBalance) in the **Predefined quantities** drop-down list.



IO Click the **Contour plot** check box and click OK.

- **II** To visualize the local conversion in selected cross sections along the length of the reactor, go to the **Postprocessing** menu and select **Cross-Section Plot Parameters**.
- **12** Click the Line/Extrusion tab.
- **I3** Enter xA in the **Expression** edit field.
- **I4** Enter 0 in the **r0** edit field and 0.1 in the **r1** edit field.
- **I5** Enter 0 in both the **z0** and **z1** edit fields.
- I6 Check the Multi parallel lines box and click the Vector with distances option.

17 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.

Cross-Section Plot Parameters
General Line/Extrusion Point
Line/Extrusion plot Plot type Une plot Line plot
y-axis data Predefined quantities:
x-axis data
✓ Multiple parallel lines Number of lines ✓ <
OK Cancel Apply

18 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 Setting	ş	X
Line color:	Cycle	Color
Line style:	Dotted line	v
Line marker:	Cycle	×
Legend		
		OK Cancel

19 To generate the following plot, click **OK** twice: first in the **Line Settings** dialog box, then again in the **Cross-Section Plot Parameters** dialog box.



Figure 2-3: Radial conversion profiles at the inlet, outlet and halfway through an adiabatic reactor.

You can now calculate the mixing cup outlet concentration (see the previous example for its definition). Start by calculating the integral of the outlet flux over the outlet boundary.

- 20 Go to the Postprocessing menu and select Boundary Integration.
- 21 Select boundary 3 in the Boundary selection list.
- 2 Enter 2*pi*r*cA*uz in the Expression edit field.
- 23 Click Apply.

The value of the integral appears in the status bar at the bottom of the user interface and reads 0.088836. You can now calculate the integral of u_z .

24 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 0.088836/5e-4, which is approximately 178 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 and perform the exercises, you can either use the results in the model just presented, or you can solve it again with new input data.

- I How do you explain the difference in outlet conversion between the isothermal and non-isothermal adiabatic reactor? (For a clue, examine the temperature plot.)
- **2** This section deals with the model of an adiabatic reactor. What is special about the solution's surface plot of the temperature? Explain the resulting radial temperature distribution.
- **3** Increase the thermal conductivity, ke, by a factor of 10 and explain how this affects the temperature profiles. At what radial position do you find the highest conversion? You can change the thermal conductivity by going to the **Options** menu and then the **Constants** item. Click the **Solve** button to solve the problem with the new thermal conductivity.



- 15. In Step 19 of page 44 in the ECRE manual (and on page 13 of 19 in this pdf file) it asked you to make a Cross-Section plot. I prefer to use as the x-axis data either the z or the r coordinate. Also in the line Settings box I always request a legend.
- 16. Also a title to the graph as well as axis labels can be specified. Select the General tap and the Title/Axis button.
- 17. This plot can now be pasted into a word document by selecting the MS windows copy icon.

Title/Axis Settings	Cross-Section Plot Parameters
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	General Line/Extrusion Point Plot type Image: Distribution of the second secon
Cross Section Plot of the Isothermal Laminar Flow reactor	Title/Axis Button
0.3	Title/Axis
0.2	
0.1 0 0 0.02 0.04 Radius (m) 0.06 0.08 0.1	OK Cancel Apply



- 18. 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.
- 19. 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.
- 20. Then start the conversion of the data using a delimited file.\

Text Import Wizard - Step 1 of 3	? 🔀							
The Text Wizard has determined that your data is Delimited. If this is correct, choose Next, or choose the data type that best 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 row: 1	File <u>o</u> rigin: 437 : OEM United States 🛛 👻							
Preview of file C:\Documents and Settings\H.	cross-sectiondata isothermal laminar.txt.							
1 Coordinates								
35.0251256E-4 -1.1	8684E-16							
40.0010050251 0.0								
<u>5</u> 0.0015075378 0.0	✓							
	>							
Ca	el < Back Next > Finish							



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	
▼ <u>Space</u> Other: Text <u>q</u> ualifier:	
-Data preview	
* Coordinates	
0.0 0.0 5 0251256R-4 -1 1368684R-16	
p.0010050251 p.0	
0.0015075378 0.0	~
Cancel < <u>B</u> ack <u>N</u> ext > <u>F</u> inis	h

21. 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.

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	A	B			-0.5m	F		A	B			0.5m
198	0.098492	0				-	198	0.098492	0			
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200	0.099497	0					200	0.099497	0			
201	0.1	0	End of data	i for z=On	n		201	0.1	0	End of dat	ta for z=Or	n
202	0	0.269076	Start of dai	a for z=0.	.5m		202	0	0.269076	Start of da	iia for z=O	.5m
203	5.03E-04	0.269081					203	5.03E-04	0.269081			
204	0.001005	0.269096					204	0.001005	0.269096			
205	0.001508	0.269121					205	0.001508	0.269121			
206	0.00201	0.269155					206	0.00201	0.269155			
400	0.099497	0.950558					598	0.098492	0.957453			
401	0.1	0.960809	End of data	for z=0.5	5		599	0.098995	0.964472			
402	0	0.424049	Start of dat	a for z=1.	.0m		600	0.099497	0.969844			
403	5.03E-04	0.424055					601	0.1	0.973568	End of dat	ta for z=1.0	Om
404	0.001005	0.424074					602	%	Elements	(triangular)	
405	0.001508	0.424105					603	1	2			
406	0.00201	0.424148					604	2	3			
407	0.002513	0.424203					605	3	4			
408	0.003015	0.424271					606	4	5			
409	0.003518	0.424352					607	5	6			
410	0.00402	0.424444					608	6	7			
411	0.004523	0.424549					609		8			
412	0.005025	0.424667					610	8	9			
413	0.005528	0.424797					011	10	10			
414 A15	0.00603	0.424939					613	10	12			
415	0.0000000	0.420094					614	12	12			
410	0.007538	0.425201					615	13	14			
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Find and	Replace	? 🔀
Find	Replace	
Fi <u>n</u> d wha	: 0.1	~
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	Find All Eind Next	Close

To be Submitted:

Submit all work in email with the subject title, "Comsol Adiabatic Reactor." All "printouts" should be pasted into a word document and submitted by email. Answer any questions using text in the word document. Place figure captions on all figures to explain what you have plotted.

- 1) POLYMATH model and requested plots
- Answer Questions 1-3 on page 14 of 19 in this tutorial (page 45 of the ECRE manual).
- 3) Reset your model to the base case conditions given in the above tutorial (Diff= 1×10^{-9} m²/s and ke = 0.559 J/m·s·K.)

Subdomain Settings - Co	nvection and Diffu	sion (MassBalanc	e)	Ζ
Equation ⊽•(-D⊽cA+cAu) = R, cA = c	oncentration			
Subdomain selection	CA Init Element			_
	Library material:		ad	
	Quantity	Value/Expression	Description	
	^ŏ ts	1	Time-scaling coefficient	
	 D isotropic 	0	Diffusion coefficient	
	🔘 D anisotropic	1001	Diffusion coefficient	
	R	rA	Reaction rate	
~	u	0	r-velocity	
	v	uO	z-velocity	
 Select by group Active in this domain 	Artificial Diffusion			
		ок	Cancel Apply	

a) Run the following cases: (Remember to change a parameter in either the mass balance or energy balance you must select it using the Multiphysics

07			
Case	Diffusivity (m^2/s)	Thermal Conductivity	Velocity Profile
		(J/(m s K)	
Base Case	1×10 ⁻⁹	0.559	$u_z = 2 * u_0 \left(1 - \left(\frac{r}{R_a} \right)^2 \right)$
Case 1	0	0.559	$u_z = u_0$
Case 2	0	0	$u_z = u_0$

- b) Compare the base case with Case 1 and Case 2. Do this using surface plots and crosssection plots of conversion and temperature.
- c) Compare Case 1 and Case 2 with your POLYMATH model results. Make plots of T and X_A vs L that show predictions of cases 1 & 2 and your POLYMATH results from a plug flow reactor.
- d) Compare the average outlet conversion and temperature from the COMSOL laminar flow adiabatic reactor model (base case) with the outlet conversions and temperatures obtained from the POLYMATH PFR. Write a statement on the comparison of the conversion of these two data sets.

Cross-Section Plot Parameters	Cross-Section Plot Parameters					
General Line/Extrusion Point	General Line/Extrusion Point					
Plot type	⊙ Line/Extrusion plot					
Line/Extrusion plot O Point plot	Plot type					
Solutions to use Solution at angle (phase):	Line plot Extrusion plot					
Select via:	y-axis data					
	Predefined quantities:					
	Expression: xA					
	Cross-section line data					
	⊙ <u>z</u> <u>v</u> r0: <u>0</u> r1: <u>0</u>					
	O Expression ZU: U Z1: 1 Line resolution: 200					
	Number of lines Vector with distances					
	5 0 0.05 0.1					
OK Cancel Apply	Line Settings Surface Settings					
In the Table for anisotropic the Diffusivitie						
are:	OK Cancel Apply					
Dr (radial)						
Dz (axia	l)					
Subdomain Settings - Convection and Diffusion (MassBalance)						
Equation $\nabla \bullet (D\nabla c A + c A u) = R \ c A = concentration$						
Subdomain selection						
	1					
Library material.						
Quantity	Value/Expression Description					
o _{ts}	1 Time-scaling coefficient					
O D isotropic	Diff Diffusion coefficient					
 D anisotropic 	0 0 0 Diff Diffusion coefficient					
R	rA 0 0					
🖌 🗸 u	0 Diff					
Select by group	u0 z-velocity					
Artificial Diffus	sion					