Revised: 11/25/03

ChE 528
Problem Set 11
Due Thursday 12/4/2003

1. Use FEMLAB to resolve the dispersion part of Example 14-1
   a) How does your FEMLAB result compare with the book? Vary the dispersion coefficient (D_a) with the lower limit being the diffusivity, D_{AB}, and write a sentence or two saying how the conversion changes.
   b) Now assume laminar flow and consider radial gradients in concentration. Use D_{AB} for both the radial and axial diffusion coefficients. Compare your results with part (a). Describe and explain your findings.
   c) Now use the open-vessel boundary condition (cA = CA0) for the inlet. Compare your results with part (b). Why is the average outlet conversion in this part lower than that in part (b)? Which boundary condition is more appropriate in this case? In what situation will the two boundary conditions result in much different outlet conversions?

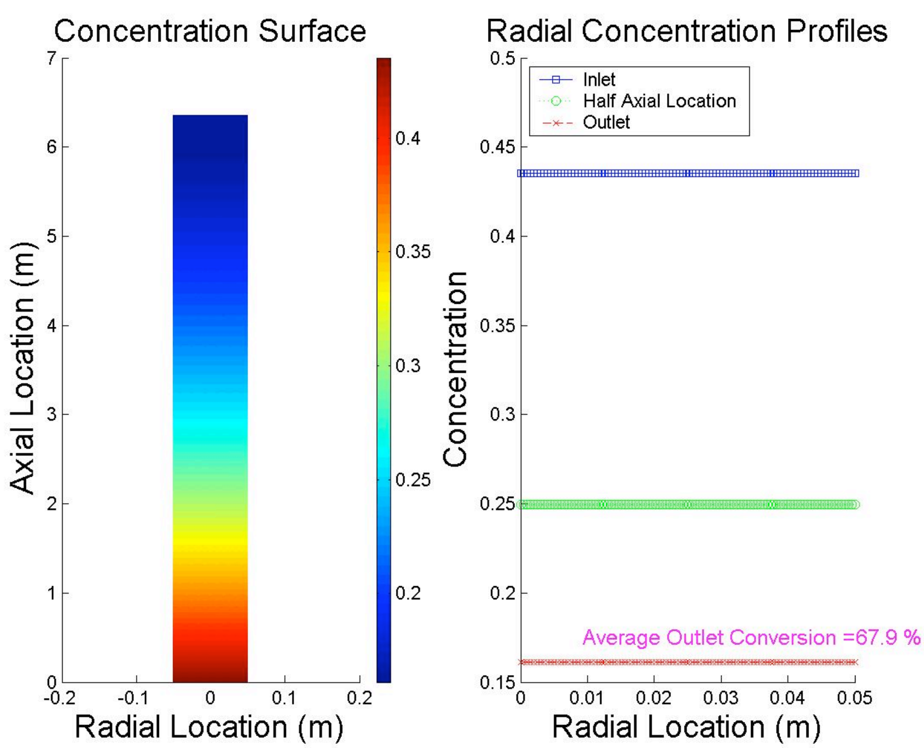
   Additional information:

   C_{A0} = 0.5 mol/dm^3, $U_0 = L/\tau$ = 1.24 m/min, $D_a = U_0{*}L/Pe_r$ = 1.05 m^2/min. D_{AB} = 7.6E-5 m^2/min.

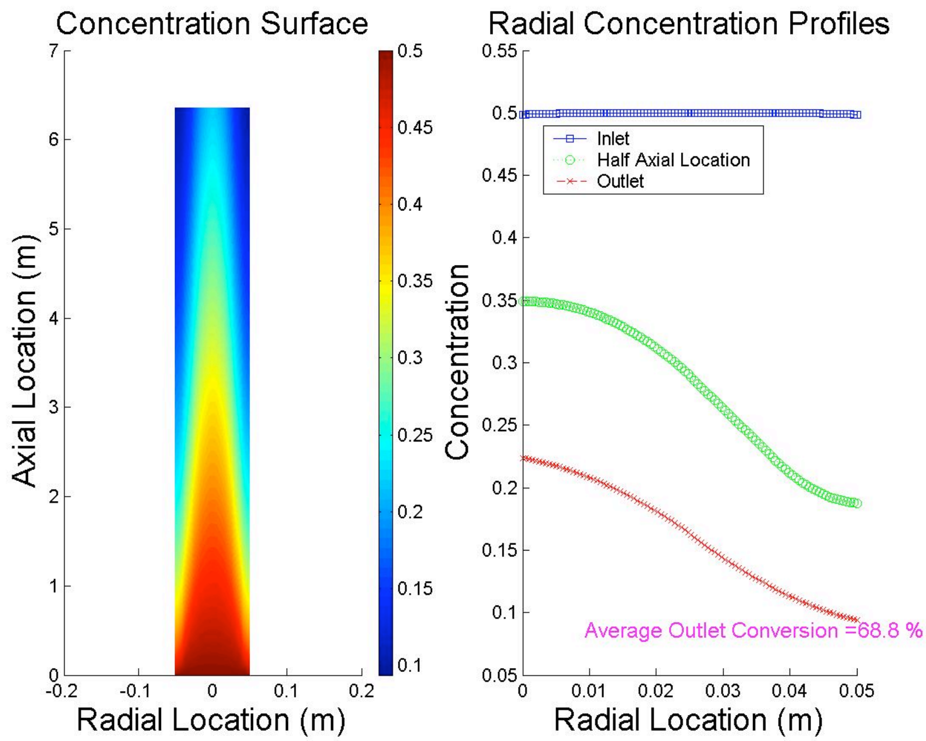
   Note: For part (a), use a plug-flow 2-D model because it is easier to extend to part (b). The inlet boundary condition for part (a) and part (b) is closed-vessel (flux($z = 0^-$) = flux($z = 0^+$) or $u_z \cdot C_{A0}$ = flux at the inlet boundary). In Femlab form:
   - Part a) $-N_i \cdot n$ = *U0*CA0*
   - Part b) $-N_i \cdot n$ = *2*U0*(1-(r/R).^2)*CA0*

   You can download the Matlab file plotcA.m from the 528 website to plot the concentration profiles and obtain the overall conversion.

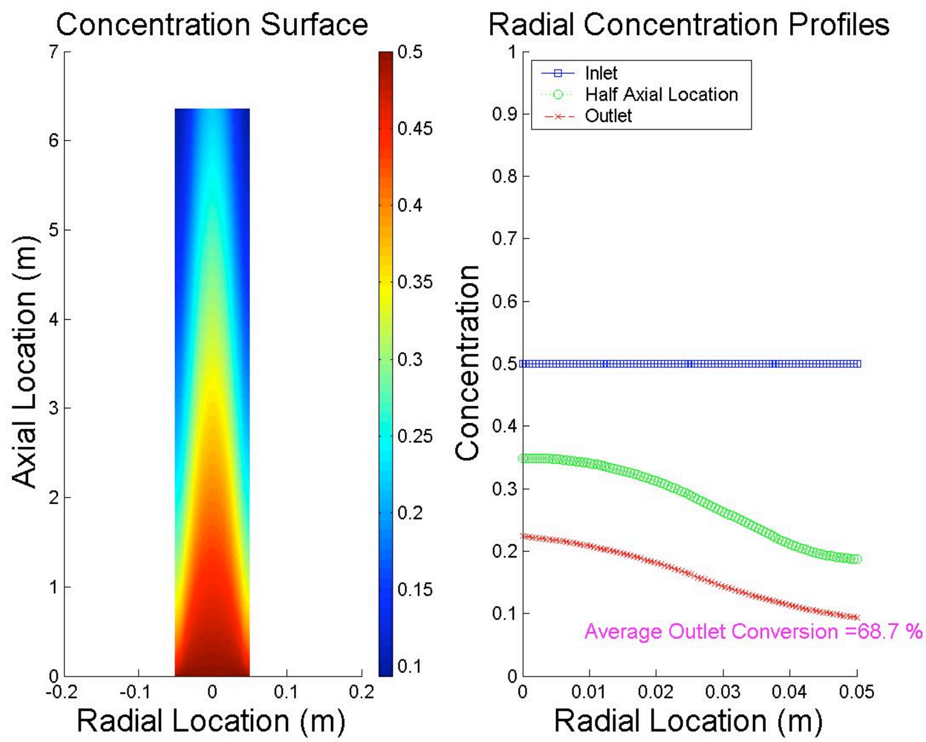
Problem 11-1 a)



Problem 11-1 b)

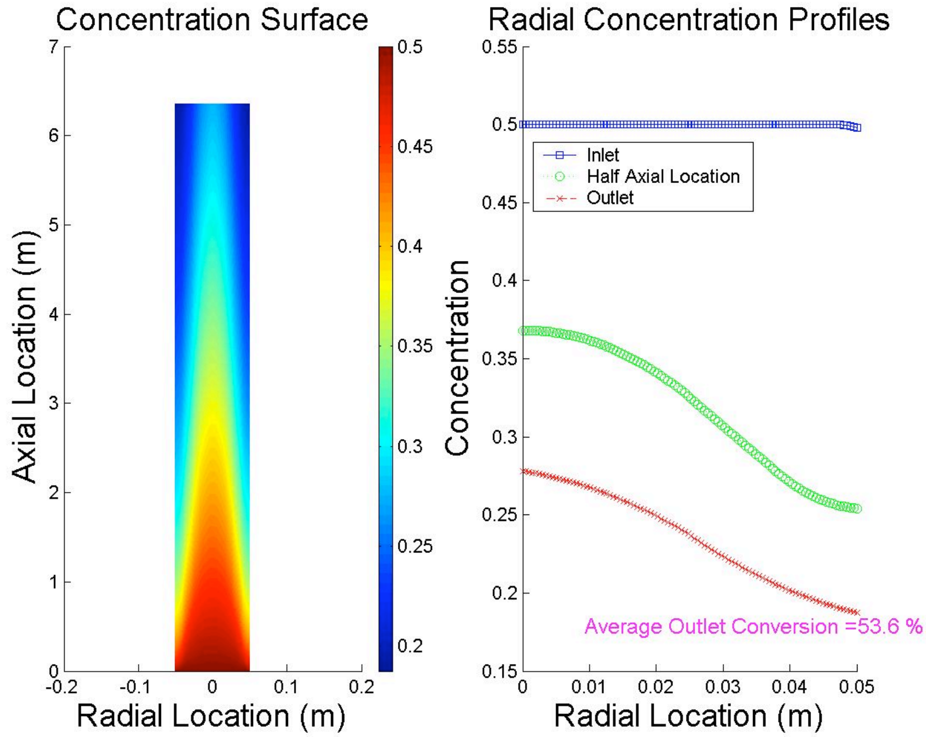


Problem 11-1 c)



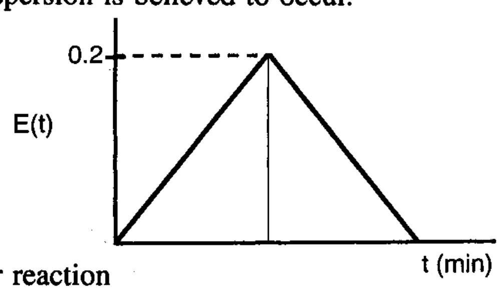
2. Expand your results in Part (b) to consider the case when the reaction is second order with $k = 0.5\ dm^3/mol \cdot min$ and $C_{A0} = 0.5\ mol/dm^3$. Assuming the radial dispersion coefficient equals to the molecular diffusivity. Vary the Peclet number (by

varying D_a) and the Damköhler number (by varying k or C_{A0}) and write a paragraph describing what you find.



3. P14-18

P14-18$_B$ The following E(t) curve was obtained from a tracer test on a tubular reactor in which dispersion is believed to occur.



A first order reaction

$$A \xrightarrow{k} B$$

is to be carreid out in the reactor. There is no dispersion occurring either upstream or downstream of the reactor but there is dispersion inside the reactor.

(a) What is the Peclet number?

(b) What is the conversion?

Additional information

$k = 0.2\ \text{min}^{-1}$

4. P14-12 (a)

P14-12$_C$ Consider a real tubular reactor in which dispersion is occurring.

(a) Show for a the first order reaction that the tanks-in-series model gives the same conversion as the maximum mixedness model for any E(t) curve. [Hint: use a Taylor series Expansion.]

5. P14-19

P14-19$_B$ The second order reaction described in Problem 14-17 is to be carried out in a real reactor which gave the following outlet concentration for a step input.

For $0 \leq t < 10$ min then $C_T = 10\ (1-e^{-.1t})$

For $10 \leq t$ then $C_T = 5+10\ (1-e^{-.1t})$

(a) What model do you propose and what are your model parameters, α and β?

(b) What conversion can be expected in the real reactor?

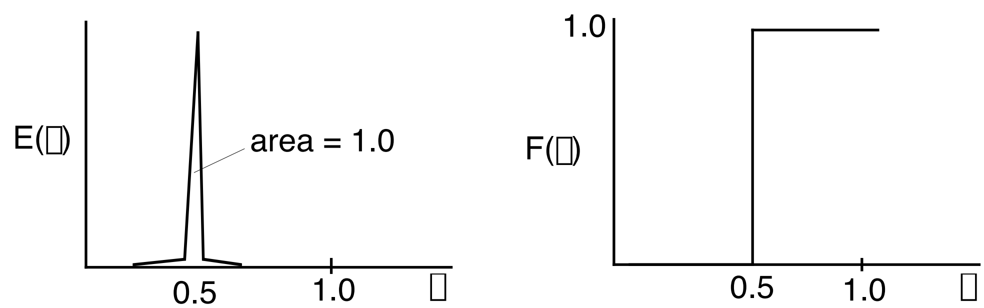
(c) How would your model change and conversion change if your outlet tracer concentration was

For $t \leq 10$ min, then $C_T = 0$

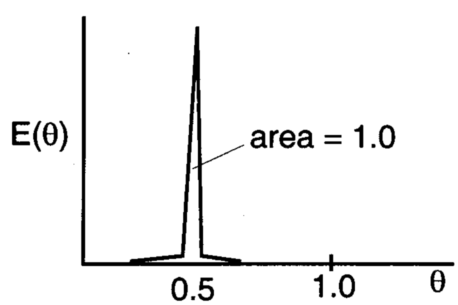
For $t \geq 10$ min, then $C_T = 5+10\ (1-e^{.2(t-10)})$

6. Suggest combinations of ideal reactors to model the following real reactors, given E(□), F(□), or 1–F(□).

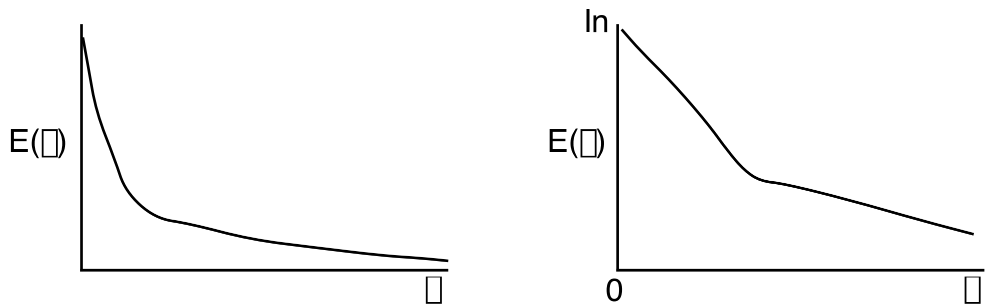
a)



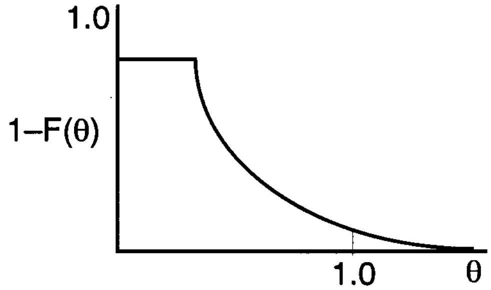
b)



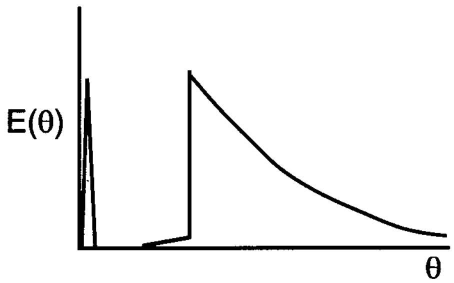
c)



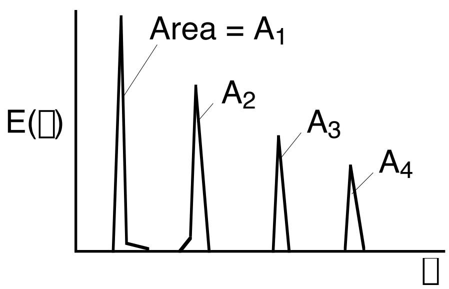
d)



e)



f)



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