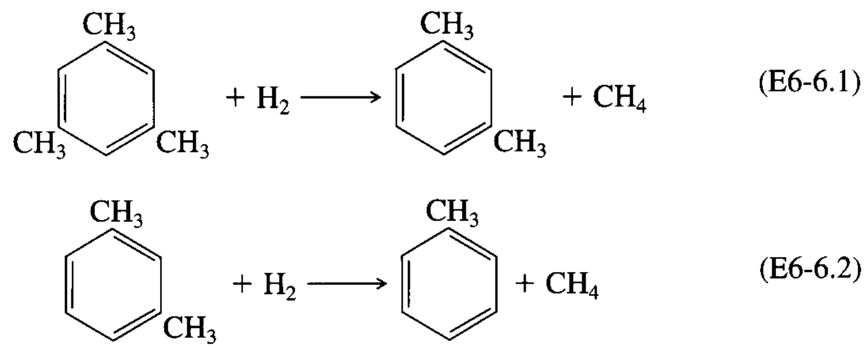
ChE 528

Problem Set 3

Due Tuesday 9/23/2003

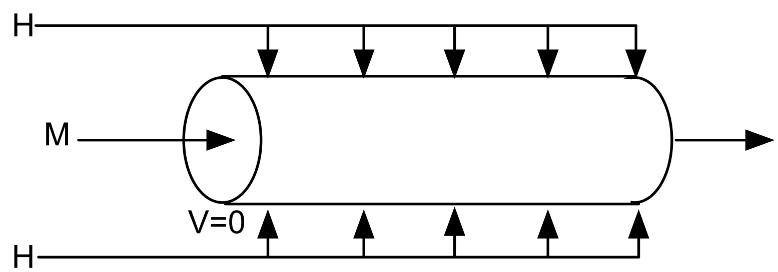
1. P6-X Now consider using a membrane reactor and feeding hydrogen uniformly through the sides of the reactor in order to compare with feeding hydrogen along with mesitylene to the entrance.



We will write symbolically as

$$M + H \rightarrow X + Me \qquad -r_M = k_1 C_M C_H^{1/2}$$

$$X + H \rightarrow Tl + Me \qquad r_{2T1} = k_2 C_X C_H^{1/2}$$



The reaction conditions and rate law of parameters are the same as described in Example 6-6. The mole fractions of mesitylene and hydrogen are to be varied but the total molar flow rate is to remain constant at 15.2 lb moles/h.

Plot the molar flow rates and selectivity of xylene to toluene as a function of catalyst weight (volume) down the reactor. Compare the selectives, $S_{X/Tl}$, and molar flow rates of xylene F_X, at the end of the reactor $V=V_T$ with the case all the hydrogen had been fed at the entrance.

This problem is open ended in that you want to suggest the best operating conditions to maximize the molar flow rate of xylene, F_X, and the selectivity, $S_{X/Tl}$.

(A) No separation cost.

Vary y_{M0} and V_T

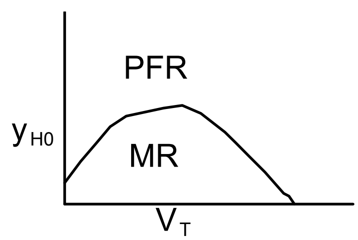
$5 \le V_T < 238\ ft^3$

$0.02 < y_{M0} \le 0.98$

Start with the conditions that are identical to Example 6-6 to find F_X and $S_{X/Tl}$. Compare these results for F_X and $S_{X/Tl}$ with those in Example 6-6 Next try an equal molar feed of mesitylene to the reactor and hydrogen to the shell side and vary the reactor length to plot $S_{X/Tl}$ and F_X vs. V_T. Once you find the best operating conditions compare them with the operation of a conventional tubular reactor.

You might even make a phase plane plot of y_{H0} vs. V_T indicating those regions where the membrane reactor is best and those where the conventional PFR is best.

e.g.,



Note: In some cases Polymath may crash because one of the variable, i.e., H_2, is small and may fluctuate to be a negative value. When polymath then tries to take the square root of a negative value it crashes. For example, for an equal molar feed, the maximum reactor volume is between 180 ft^3 and 200 ft^3. For a final volume above that the molar flow rate of hydrogen becomes too small.

(B) Separation costs Vary y_{M0} and V_T

You are to construct a cost function. Examples of cost functions might be

(1) $ profit = $\$_1 F_X - \$_2 F_{T\ell} - \$_3 F_{H0} - \$_4 F_{M0} - \$_{OP}$, with $\$_1$ = \$400/mol, etc. and $\$_{OP}$ the fixed and operating costs.

or

(2) $ Profit = $\$_1 S_{XY} - \$_{OP}$

or a continuation of (1) and (2)

However, the choice is yours, but you must write a few sentences justifying your reasoning

2. Problem 7-7 (a), (c), and (f). For part (f) only do the low temperature pathways.
3. Problem 8-8 (a) and (b)

(a) **Plot the temperature and conversion profiles for a PBR with:**

$$\frac{Ua}{\rho_b} = 0.8 \frac{\text{J}}{\text{s} \cdot \text{kg cat.} \cdot \text{K}}$$

where

ρ_b = bulk density of the catalyst (kg/m^3)

a = heat-exchange area per unit volume of reactor (m^2/m^3)

U = overall heat-transfer coefficient (J/s · m^2 · K)

(b) **What are the profiles if Ua/ρ_b were increased by a factor of 25? of 10?**

4. Problem 8-15 (a through f). But……Save Paper!!! Print out only two or plots for each (a) and (b) and **only** then sketch and describe the trends when you vary each the parameters in parts (a) through (f). Read through the corresponding self test workbook on the web in Chapter 8.

5. Calculate the frequency factor, A using collision theory for the following reactions at 0°C

		(Experimental)[†] A(Å^3/molecule•s)
(1)	$H + C_2H_6 \rightarrow C_2H_5 \bullet\ H_2$	1.6 x 10^{14}
(2)	$F + H_2 \rightarrow HF + H$	
(3)	$CO + O \rightarrow CO_2$	
(4)	$O_2 + H \rightarrow OH + O$	1 x 10^{13}
(5)	$O + C_2H_6 \rightarrow OH + C_2H_5$	2.5 x 10^{13}

[†]Westley, F., *Table of Recommended Rate Constants for Chemical Reactions Occurring in Combustion*, NBS, Washington DC (1980)

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6. Plot the distribution energy distribution f(E,T) function as a function of E for T=300K and for T=600K for the reaction. For an activation energy of 3 Kcal, calculate the fraction of collisions that have energy above 3 Kcal/mol and react at each temperature.

7. Turn in a copy of the journal article you plan to critique along with a typed half page outline of three challenges you will make and a description of how you will use critical thinking in analyzing the article you have chosen.