ChE 321: Kinetics and Reactor Designs (Spring 2011)
Exam Two (Closed Book and Closed Notes)

NAME: Key

Problem 1. Short Answer Questions. [30 pts]

(a) A reversible water gas shift (WGS) reaction can be written as following:

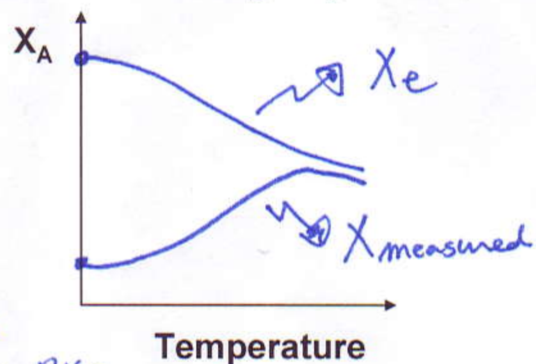
→ [15 pts]

$$CO + H_2O \underset{K_{-A}}{\overset{K_A}{\rightleftharpoons}} CO_2 + H_2$$

It is an exothermic reaction with ΔG^o_{Rxn} = -730 cal/mol. Please draw following two plots on a single graph:

(i) Equilibrium conversion Vs. reactor temperature

(ii) True or measured conversion Vs. reactor temperature



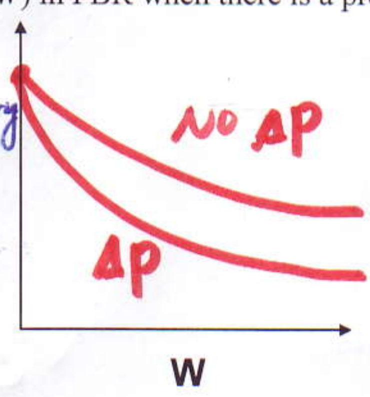
Please briefly justify the shapes of your plots.

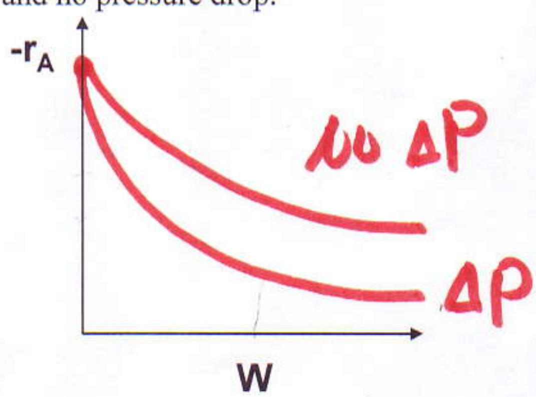
- X_e ↓ as Temp ↑ b/c equil. shifts to left as temp ↑ for the exothermic RXN.
- $X_{measured}$ ↑ as temp ↑ b/c the kinetic improves as temp ↑ according to Arrhenius Eq.

(b) A gas phase reaction occurs in an ideal PBR: A → B. Please draw plots of concentration of A (C_A) vs. weight of catalysts (W) in PBR when there is a pressure drop and no pressure drop. Then, draw plots of the rate of disappearance of A ($-r_A$) vs. weight of catalysts (W) in PBR when there is a pressure drop and no pressure drop.

[15 pts] ←

Elementary





Comparing two reactor designs where the first reactor has a significant press drop & the second reactor has no pressure drop, which design would require less amount of catalyst to achieve 90% conv. of A ?? → "The reactor design with no ΔP !!!"

Problem 2: This is a selectivity problem for a reactor design with multiple reactions [25Pts]

Please consider following two multiple reactions

$$A + B \rightarrow D \quad \textbf{(Reaction 1)}$$
$$A + B \rightarrow U \quad \textbf{(Reaction 2)}$$

The rate laws for reactions (1) and (2) are:

$$-r_1 = 200{,}000 * \mathrm{Exp}(-8{,}000/T) * P_A^{3} * P_B \qquad \text{(Reaction 1)}$$

$$-r_2 = 500 * \mathrm{Exp}(-2{,}000/T) * P_A * P_B^{4} \qquad \text{(Reaction 2)}$$

(T is in Kelvin)

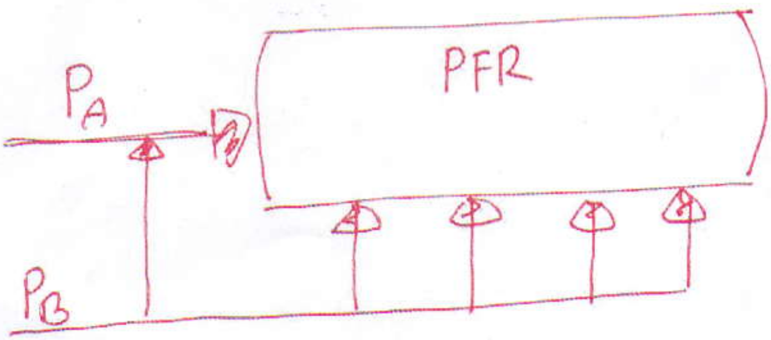
(i.e. Partial pressures of A & B, and reactor temp)

Where P_A and P_B are the partial pressure of A and B. Please describe a ***flow reactor*** design that can maximize the selectivity of D over U. To receive a full credit, you need to (i) draw the reactor, (ii) briefly describe its operating conditions and (iii) support your reactor design based the mathematical expression of its selectivity (i.e. $S_{D/U}$).

$$S_{D/U} = \frac{\overset{400}{\cancel{200{,}000}}\ \mathrm{Exp}(-8{,}000/T)\ P_A^{\cancel{3}\,2}\ \cancel{P_B}}{\cancel{500}\ \mathrm{Exp}(-2{,}000/T)\ \cancel{P_A}\ P_B^{\cancel{4}\,3}} \quad [5\text{Pts}]$$

$$= 400\,\mathrm{EXP}(-6{,}000/T)\ \frac{P_A^2}{P_B^3}$$

∴ To ↑ $S_{D/U}$, ① Keep P_A high, ② keep P_B Low, & ③ use high temp.



- Use a side stream of B so that we can maintain the P_B low while keeping the P_A high.
- Keep the Reactor temp high, but Not too high to keep the reactor from melting.

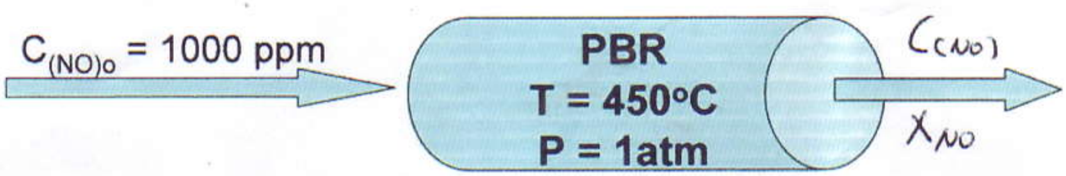
[20Pts]

Problem 3: Differential analysis of rate data [45 PtS]

Automotive emissions of nitrogen oxides are typically controlled by means of a "three-way" converter located in the exhaust train in which more than 95% of the CO and hydrocarbons are oxidized and 95% of the NO is simultaneously reduced by CO and hydrocarbons:

$$2\,CO + 2\,NO \rightarrow N_2 + 3\,CO_2$$

The NO reduction catalyst is most generally Pt-Rh nanoparticles on Al_2O_3 support, which has been wash-coated on a ceramic, honeycomb monolith. To simplify the problem, one can assume this honeycomb monolith reactor as an ideal pack bed reactor.

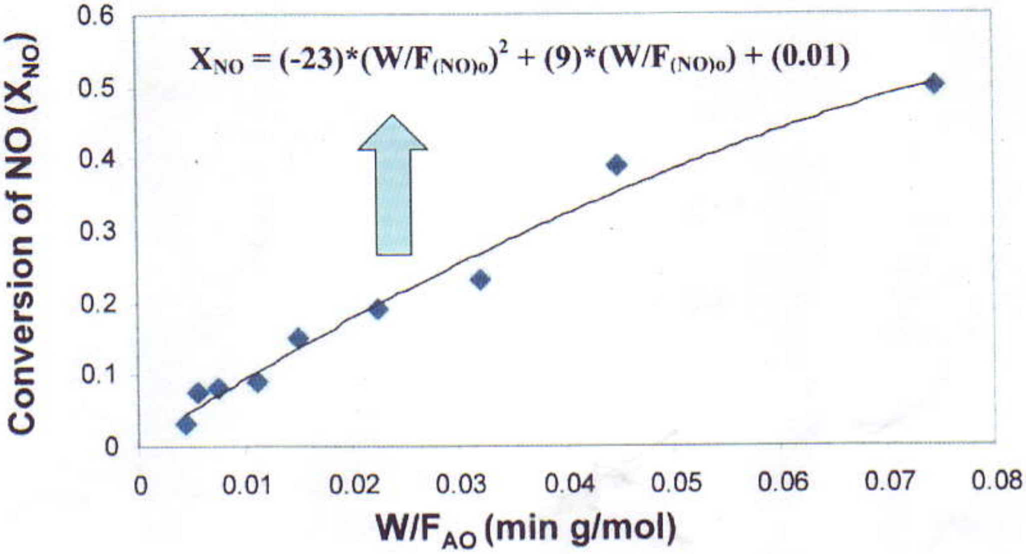


The following rate data for NO reduction of CO were obtained in an ideal pack bed reactor with 1 g of Pt-Rh/Al_2O_3 catalysts. It will be assumed that rates were measured at 1 atm total pressure and 450°C using a simulated exhaust containing 1000 ppm NO, 2% CO, 1% O_2, 10% CO_2, 10% H_2O, and balanced N_2.

vo (cm^3/min)	$W/F_{(NO)o}$ (min g/mol)	C_{NO} (ppm)	X_{NO}
300	0.0500	590	0.5820
500	0.0448	610	0.3900
700	0.0320	720	0.2300
1000	0.0224	810	0.1900
1500	0.0149	850	0.1500
2000	0.0112	910	0.0900
~~3000~~	~~0.0075~~	~~920~~	~~0.0800~~
~~4000~~	~~0.0056~~	~~925~~	~~0.0750~~
5000	0.0045	968	0.0320

Values of X_{NO} (*conversion of NO*) are plotted against $W/F_{(NO)o}$ (*Weight of catalysts/Molar flow rate of NO at inlet stream*) and the data are fitted to a simple quadratic:

$$X_{NO} = (-23)*(W/F_{(NO)o})^2 + (9)*(W/F_{(NO)o}) + (0.01)$$



Design equation of an ideal PBR can be written as following:

$$\frac{dX_{NO}}{d(W/F_{(NO)o})} = -r_{NO}$$

Previous researchers have shown that the rate of disappearanc of NO ($-r_{NO}$) follows a simple power law:

$$-r_{NO} = k*(C_{NO})^{\alpha}$$

Where k is a rate constant, C_{NO} is concentration of NO and α is reaction order.

(a) Based on given rate data information and design equation of an ideal PBR, please estimate both the rate constant and reaction order using the differential analysis method. In order to receive a full credit, please clearly show following items:

(i) How to estimate the rate of disappearance of NO ($-r_{NO}$) at different values of $W/F_{(NO)o}$ using given rate data and differential analysis method [30 PTS]

(ii) Plot the figure with clearly labeled x-axis and y-axis and show how to estimate the values of both rate constant and reaction order [15 PTS]

$$-r_{NO} = K\,(C_{NO})^{\alpha}$$

+3

$$\underbrace{\ln(-r_{NO})}_{y} = \underbrace{\ln K}_{b} + \underbrace{\alpha}_{m}\,\underbrace{\ln(C_{NO})}_{x}$$

$$y = b + m \cdot x$$

Now, we need to estimate the value of $-r_{NO}$ using the diff method.

↳ To do it, we need to find a diff expression that allows us to calc. the value of $-r_{NO}$ using the given rate data.

Design Eq of Ideal PBR $\Rightarrow$ $F_{(NO)_0} \dfrac{dX_{NO}}{dW} = -r_{NO}$

$$\underbrace{\frac{dX_{NO}}{d(W/F_{(NO)_0})}} = -r_{NO}$$

Need to diff. X_{NO} respect to $W/F_{(NO)_0}$

$$\underbrace{X_{NO}}_{y} = (-23)\underbrace{(W/F_{(NO)_0})}_{x}^2 + (9)\underbrace{(W/F_{(NO)_0})}_{x} + (0.01)$$

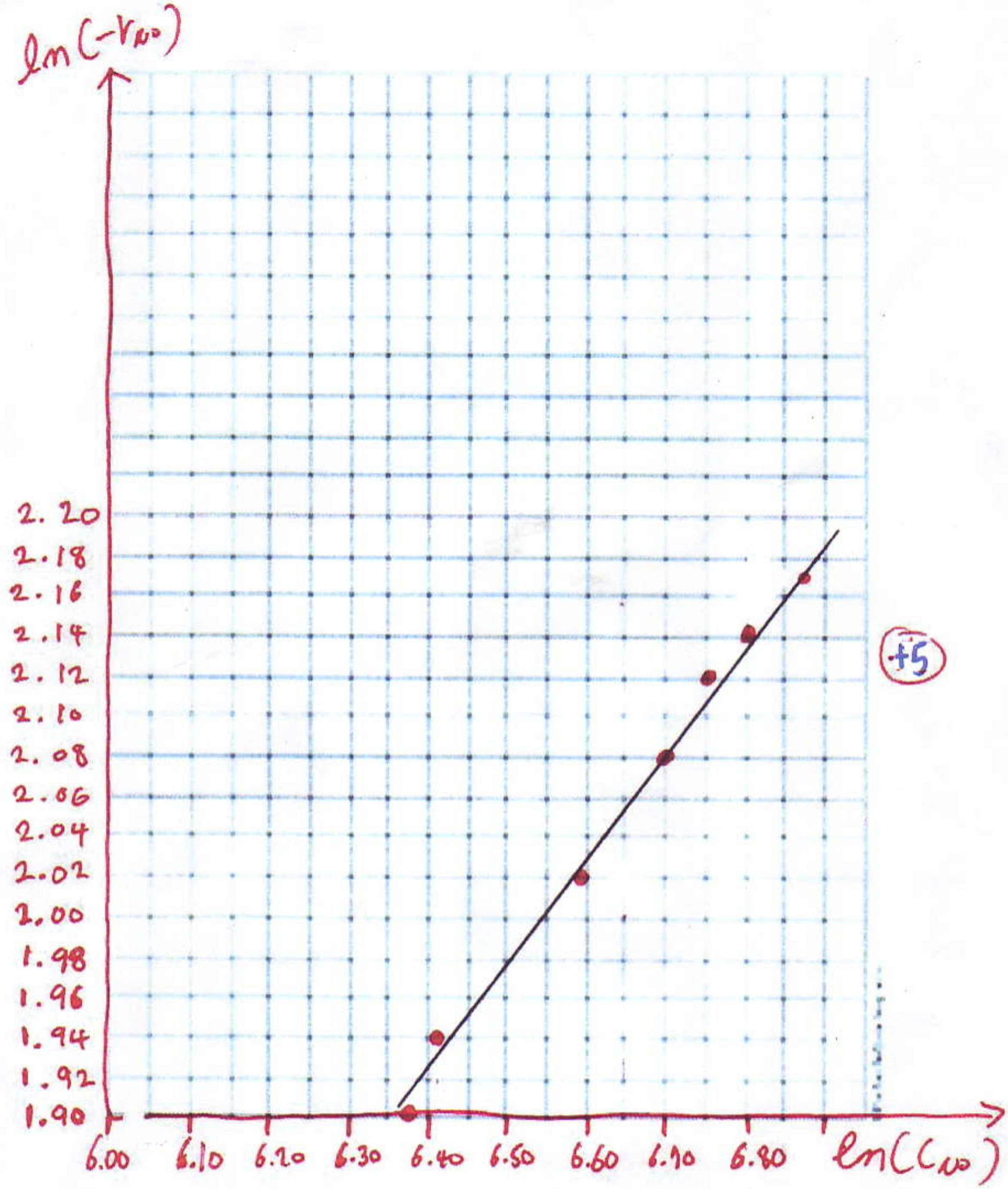
$$\frac{dX_{NO}}{d(W/F_{(NO)_0})} = \frac{dy}{dx} = (-46)x + 9$$ +15

$W/F_{(NO)_0}$	C_{NO}	$-r_{NO}$	$\ln(C_{NO})$	$\ln(-r_{NO})$
0.05	590	6.70	6.38	1.90
0.0448	610	6.94	6.41	1.94
0.032	720	7.53	6.58	2.02
0.0224	810	7.97	6.70	2.08
0.0149	850	8.31	6.75	2.12
0.0112	910	8.48	6.81	2.14
~~0.0075~~	~~920~~	~~8.66~~	~~6.82~~	~~2.16~~
~~0.0056~~	~~925~~	~~8.74~~	~~6.83~~	~~2.17~~
0.0043	968	8.79	6.88	2.17

+10

delet!!

1.14
.5



(+5)

$$\text{Slop} = \alpha = \frac{(1.90 - 2.08)}{(6.35 - 6.70)} = \boxed{0.51}$$ (+5)

$$2.08 = \ln K + (0.51)(6.70)$$

$$\ln K = (2.08) - (0.51)(6.70) = -1.337$$ (+5)

$$\boxed{K = 0.26}$$