

## ChE 7033 Homework 2 due September 23, 2004

Each problem is worth 33%

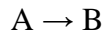
1. The gas phase reaction:



takes place in a constant volume batch reactor. Addition of B or C to the reaction mixture has no effect on the rate of the reaction. Several reaction runs have been performed at different initial partial pressures and different temperatures and the results are tabulated below. From this data, find a suitable LHHW rate expression that fits the data. Evaluate all parameters for the rate expression including  $K$ 's (equilibrium adsorption constants) for all the components,  $\lambda$ 's ( heats of adsorption), and  $E$  (the true activation energy).

Rxn Time (min)	T = 400 K		T = 410 K	T = 390 K
	$P_A$ (atm)	$P_A$ (atm)	$P_A$ (atm)	$P_A$ (atm)
0	1.00	2.00	1.00	1.00
10	0.79	1.68	0.52	0.92
20	0.62	1.39	0.25	0.85
40	0.36	0.90	0.05	0.72
60	0.20	0.55	0.01	0.61

2. Consider a simple irreversible, catalytic isomerization reaction:



We would like to determine a suitable rate expression, so we gather rate data in a constant volume batch reactor. Assume ideal gases, surface reaction rate controlling.  $T$  is constant at 300K.

Run #	$-r_A$ (moles/lit-min)	$P_A$ (torr)	$P_B$ (torr)
1	$3.529 \times 10^{-3}$	100	200
2	$6.316 \times 10^{-3}$	200	200
3	$8.571 \times 10^{-3}$	300	200
4	$10.435 \times 10^{-3}$	400	200
5	$7.273 \times 10^{-3}$	200	100
6	$6.316 \times 10^{-3}$	200	200
7	$5.581 \times 10^{-3}$	200	300
8	$5.000 \times 10^{-3}$	200	400

Find a suitable LHHW rate expression and determine numerical values for each constant. How long would be required to convert 80% of the A if  $P_{A0} = 200$  torr,  $P_{B0} = 0$  torr,  $T = 300K$ , and the reaction is carried out in an isothermal batch reactor?

3. Do Problem 3.1 in Froment and Bischoff