

ChE 321: Kinetics and Reactor Design
HW#4
(Due 2/16/2011)

1. The gas phase reaction,



Is to be carried out isothermally using CSTR. The molar feed is 50% H₂ and 50% N₂, at a pressure of 16.4 atm and 227°C.

- (a) Construct a complete stoichiometric table by taking H₂ as your basis of calculation.
- (b) What are C_{A0}, δ and ε? Calculate the concentration of ammonia and hydrogen when the conversion of H₂ is 60%.
- (c) Suppose by chance the reaction is elementary ($-r_{\text{N}_2} = k_{\text{N}_2} * (\text{C}_{\text{N}_2})^{0.5} * (\text{C}_{\text{H}_2})^{1.5}$) with $k_{\text{N}_2} = 40 \text{ dm}^3/\text{mol}\cdot\text{s}$. Write the rate of reaction solely as a function of conversion of H₂.

2. At 650°C, gas A decomposes as follows;



Gas A is fed to a plug flow reactor using a feed stream that contains 67% A and 33% inert. The rate equation is express as: $-r_A = (10\text{hr}^{-1})C_A$

- (a) What volume of reactor would be needed to produce 18 mole/hr of D with a 75% conversion of A? Assume that the reactor is operated under constant temperature and pressure at 650°C and 11.4 atm. Also assume that ideal gas law applies.
- (b) Draw the Levenspiel Plot using EXCEL. Base the Levenspiel Plot, *approximate* the necessary volume of reactor would be needed to produce 18 mole/hr of D with a 75% conversion of A (*In order to receive a full credit, please show how you estimate the area*).

3. Do the parts (a) and (b) of Problem P4-6B from your textbook.

4. Do the parts (a) and (b) of Problem P4-7A from your textbook.

The gas-phase reaction



is carried out isothermally in a 20-dm³ constant-volume batch reactor. Twenty moles of pure A is initially placed in the reactor. The reactor is well mixed.

(a) If the reaction is first order:

$$-r_A = kC_A \quad \text{with } k = 0.865 \text{ min}^{-1}$$

calculate the time necessary to reduce the number of moles of A in the reactor to 0.2 mol. (*Note:* $N_A = C_A V$) (*Ans.:* $t = 5.3 \text{ min}$)

(b) If the reaction is second order:

$$-r_A = kC_A^2 \quad \text{with } k = \frac{2 \text{ dm}^3}{\text{mol} \cdot \text{min}}$$

calculate the time necessary to consume 19.0 mol of A.

(c) If the temperature is 127°C, what is the initial total pressure? What is the final total pressure assuming the reaction goes to completion?