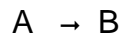


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TERM TEST - CHE218S - 1 February 2008

Please place your answers to the questions in the boxes provided. Show your work on the test paper. Answers without supporting calculations may be rejected. You may use the reverse of the previous pages if you need.

Question 1. A gas phase reaction is catalyzed by a solid catalyst.



Given: $r = k * P_A * P_B^{-1}$
 $k(250^\circ\text{C}) = 0.4 \text{ mol h}^{-1} \text{ kg}_{\text{CATALYST}}^{-1}$

1a. [5 marks] What amount of catalyst in kilograms would be required to achieve 90% conversion of a stream of 20 mol h^{-1} of pure A at 20 bar pressure at 250°C in a PFR reactor?

1b. [5 marks] . What amount of catalyst would be required to achieve the same conversion under the same conditions in a CSTR?

1c. [5 marks] The Arrhenius "activation energy" for this reaction is 145 kJ/mol . What amount of catalyst would be required in a PFR reactor at 300°C ?

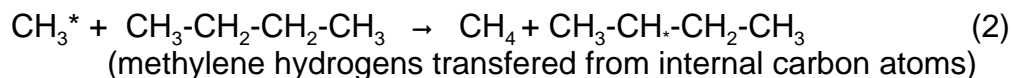
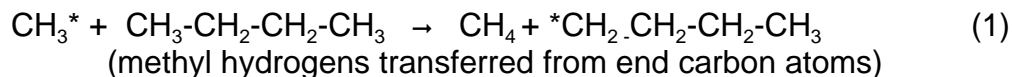
Answers to question 1

Question 1a.	_____ 70.13 _____ kg
Question 1b.	_____ 405 _____ kg
Question 1c.	_____ 3.83 _____ kg

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Question 2: [10 marks] Collision theory

Consider the two elementary reactions:



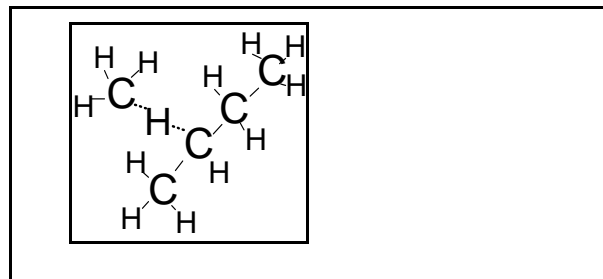
The rate constants for these two reactions are:

$$k_1 = 2.67 \times 10^{11} \exp(-7455/T(\text{K})) \text{ L mol}^{-1} \text{ s}^{-1}$$
$$k_2 = 1.28 \times 10^{11} \exp(-6750/T(\text{K})) \text{ L mol}^{-1} \text{ s}^{-1}$$

2a [5 marks] . According to the hard-spheres collision theory, what is the value of p_1/p_2 (ratio of the steric factor for reaction 1 to that for reaction 2)?

p_1/p_2 _____ 2.09 _____

2b. [2 marks] Draw an approximate transition state structure for reaction 2.



True or false:

2c. [1 mark] The transition state potential energy, E^\ddagger , is the minimum energy required for reaction. *T/F?* ___T___

2d. [1 mark] The transition state potential energy, E^\ddagger , is exactly the same as the measured "activation energy", E_A , in the Arrhenius expression. *T/F?* ___F___

2e. [1 mark] At thermal equilibrium, the ratio of the number of molecules in energy state E_1 to that in state E_2 is equal to $\exp\{(E_2 - E_1)/k_B T\}$. *T/F?* ___T___

SOLUTION

1a. PFR mass balance

$$dF_A \text{ (mol/h)} = r_A \text{ (mol kgCAT}^{-1} \text{ h}^{-1}) * d \text{ mCAT (kgCAT)}$$

Substitute rate of species for rate of reaction $r_A = -r_{\text{REACTION}}$

$$dF_A = -r_{\text{REACTION}} * d \text{ mCAT}$$

Substitute rate of species for rate of reaction $r_A = -r_{\text{REACTION}}$

$$dF_A = -0.4 (P_A/P_B) * d \text{ mCAT}$$

Substitute $P_A/P_B = F_A/F_B$ - no need for gas law, etc.

$$dF_A = -0.4 (F_A/F_B) * d \text{ mCAT}$$

Substitute $F_B = F_{A,0} - F_A$ (by mass balance, ICE table, etc.)

$$dF_A = -0.4 F_A / (F_{A,0} - F_A) * d \text{ mCAT}$$

Separate variables

$$dF_A (F_{A,0} / F_A) - dF_A = -0.4 d \text{ mCAT}$$

Integrate

$$F_{A,0} \ln(F_A / F_{A,0}) - (F_A - F_{A,0}) = -0.4 \text{ mCAT}$$

$$F_{A,0} = 20 \text{ mol h}^{-1}; F_A = 2 \text{ mol h}^{-1}$$

$$20 * \ln(0.1) - (2 - 20) = -0.4 \text{ mCAT}$$

$\text{mCAT} = 70.13 \text{ kg}$

1b. CSTR mass balance

$$\Delta F_A \text{ (mol/h)} = r_A \text{ (mol kgCAT}^{-1} \text{ h}^{-1}) * \text{mCAT (kgCAT)}$$

Substitute rate of species for rate of reaction $r_A = -r_{\text{REACTION}}$

$$\Delta F_A = -r_{\text{REACTION}} * \text{mCAT}$$

Substitute rate of species for rate of reaction $r_A = -r_{\text{REACTION}}$

$$\Delta F_A = -0.4 (P_A/P_B) * \text{mCAT}$$

Substitute $P_A/P_B = F_A/F_B$ - no need for gas law, etc.

$$\Delta F_A = -0.4 (F_A/F_B) * \text{mCAT}$$

Substitute $F_B = F_{A,0} - F_A$ (by mass balance, ICE table, etc.) and $\Delta F_A = F_A - F_{A,0}$

$$F_A - F_{A,0} = -0.4 F_A / (F_{A,0} - F_A) * \text{mCAT}$$

$$F_{A,0} = 20 \text{ mol h}^{-1}; F_A = 2 \text{ mol h}^{-1}$$

$$-18 = -0.4 * 2 / 18 * \text{mCAT}$$

$$m_{CAT} = 405 \text{ kg}$$

1c.

Arrhenius equation: $k = A \exp(-E_A / RT)$

$E_A = 145,000 \text{ J/mol}$:

$$k(250C) = A \exp(-145,000 / 8.314 (250+273.15))$$

$$k(300C) = A \exp(-145,000 / 8.314 (300+273.15))$$

$$k(300C) / k(250C) = \exp(-145,000 / 8.314 (300+273.15)) / \exp(-145,000 / 8.314 (250+273.15))$$

$$k(300C) / k(250C) = 18.32$$

since $k(250C) = 0.4$, then $k(300C) = 7.33$:

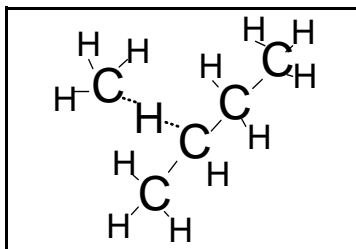
Substitute 7.33 into solution for 1a. in place of 0.4, or realize that since m_{CAT} is the basis for the reaction, $(1/18.32) \times 70.13 = 3.83 \text{ kg}$ of catalyst will provide the same rate at 300C as 70.13 kg provides at 250C. In either case:

$$m_{CAT} = 3.83 \text{ kg}$$

:

$$2a: \quad p_1/p_2 = A_1/A_2 = 2.67 \times 10^{11} / 1.28 \times 10^{11} = 2.09$$

2b: any of 4 secondary H atoms



2c: True

2d: False

2e: True