Workshop 03: Rate law and stoichiometry

Lecture notes for chemical reaction engineering

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2024-03-10

Try following problems from Fogler 5e(Fogler 2016).

P3-5, P3-10, P3-11, P3-12, P 4-6, P 4-8, P 4-11

We will go through some of these problems in the workshop.

P 3.12

Write the rate law for the following reactions assuming each reaction follows an elementary rate law. Give the units of k_A for each, keeping in mind some are homogeneous and some reactants are heterogeneous.

1. $C_2H_6 \longrightarrow C_2H_4\ H_2$
2. $C_2H_4 + \frac{1}{2} O_2 \longrightarrow C_2H_4O$
3. $(CH_3)_3COOC(CH_3)_3 \rightleftharpoons C_2H_6 + 2\,CH_3COCH_3$
4. $nC_4H_{10} \rightleftharpoons iC_4H_{10}$
5. $CH_3COOC_2H_5 + C_4H_9OH \rightleftharpoons CH_3COOC_4H_9 + C_2H_5OH$
6. $2\,CH_3NH_2 \underset{cat}{\rightleftharpoons} (CH_3)_2NH + NH_3$
7. $(CH_3CO)_2O + H_2O \rightleftharpoons 2\,CH_3COOH$

P3-10

The initial reaction rate for the elementary reaction $2\,A + B \longrightarrow 4\,C$ was measured as a function of temperature when the concentration of A was 2 M and that of B was 1.5 M.

$-r_A (mol/dm^3 s)$	$T(K)$
0.002	300
0.046	320
0.72	340
8.33	360

1. What is the activation energy?
2. What is the frequency factor?
3. What is the rate constant as a function of temperature using Equation 1 and T_0 = 27 °C as the base case?

$$k(T) = k(T_0) exp\left[\frac{E}{R}\left(\frac{1}{T_0} - \frac{1}{T}\right)\right] \tag{1}$$

P 4-8

The gas-phase reaction

$$\frac{1}{2}\,N_2 + \frac{3}{2}\,H_2 \longrightarrow NH_3$$

is to be carried out isothermally first in a flow reactor. The molar feed is 50% H_2 and 50% N_2 , at a pressure of 16.4 atm and at a temperature of $227\,^{\circ}C$?.

(a) Construct a complete stoichiometric table.

(b) Express the concentrations in mol/dm^3 of each for the reacting species as a function of conversion. Evaluate C_{A0}, δ and ϵ, and then calculate the concentrations of ammonia and hydrogen when the conversion of H_2 is 60%.

(c) Suppose by chance the reaction is elementary with $k_{N_2} = 40\ dm^3/mol/s$. Write the rate of reaction solely as a function of conversion for

(1) a flow reactor, and for

(2) a constant-volume batch reactor.

P 4-11

Consider a cylindrical batch reactor that has one end fitted with a frictionless piston attached to a spring (See Figure Figure 1). The reaction

$$A + B \longrightarrow 8\,C$$

with the rate law

$-r_A = k_1 C_A^2 C_B$

is taking place in this type of reactor.

(a) Write the rate law solely as a function of conversion, numerically evaluating all possible symbols.

(b) What is the conversion and rate of reaction when $V = 0.2\ ft^3$?

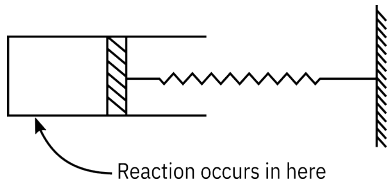

Figure 1: Cylindrical batch reactor

Additional information:

Equal moles of A and B are present at t_0

Initial volume: $0.15\ ft^3$

Value of k_1 : $1.0\ (ft^3/lbmol)^2 \cdot s^{-1}$

The spring constant is such that the relationship between the volume of the reactor and pressure within the reactor is

$V = (0.1)\ (P)$ (V in ft^3 , P in atm)

Temperature of system (considered constant): $140\ {}^\circ F$

Gas constant: $0.73\ ft^3 atm/lbmol \cdot^\circ R$

Fogler, H. Scott. 2016. *Elements of Chemical Reaction Engineering*. Fifth edition. Boston: Prentice Hall.