BT209

Bioreaction Engineering

01/02/2023

Problem 1

The first-order reversible liquid reaction A to R, (C_{A0}=0.05 mol/L, C_{R0}=0) takes place in a batch reactor. After 8 minutes, conversion of A is 33.3% while equilibrium conversion is 66.7%. Find the rate equation for this reaction.

Solution: Problem 1

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Solution X_A=0.333, X_{Ae}=0.667,

$$-\ln\left(1-\frac{X_A}{X_{Ae}}\right)=\frac{\mathrm{M}+1}{M+X_{Ae}}=k_1 t$$

M=0/0.05=0, k_1=0.05779 min-1, kc=k_1/k_2= $(M+X_{Ae})/(1-X_{Ae})$, k_2=k_1/2=0.028895 min-1

$-r_A$(mol/l.min) =0.05775 (min^{-1}) C_A (mol/l)-0.02887 (min^{-1}) C_R (mol/l)

Problem 2

In a homogeneous isothermal liquid polymerization, 20% of the monomer disappears in 34 minutes for initial monomer concentration of 0.04 and also for 0.8 mollliter. What rate equation represents the disappearance of the monomer?

Solution: Problem 2

Since the fractional disappearance is independent of initial concentration we have a first order rate, or

$$-\frac{dC}{dt} = kC \quad \cdots \text{ or } \cdots \quad \ln\frac{C_0}{C} = kt \quad \cdots \text{ where } C = \text{monomer concentration}$$

We also can find the rate constant. Thus replacing values

$$\ln\frac{C_0}{0.8C_0} = k(34\text{ min}) \quad \cdots \text{ or } \quad k = \frac{-\ln 0.8}{34\text{ min}} = 0.00657\text{ min}^{-1}$$

Hence the rate of disappearance of monomer is given by

$$-r = -\frac{dC}{dt} = (0.00657\text{ min}^{-1})C \longleftarrow$$

Problem 3

For the elementary reactions in series

$$A \xrightarrow{k_1} R \xrightarrow{k_2} S, \quad \boxed{k_1=2k_2} \quad \text{at } t = 0 \quad \begin{cases} C_A = C_{A0}, \\ C_{R0} = C_{S0} = 0 \end{cases}$$

find the maximum concentration of R and when it is reached.

Problem 4

Aqueous A at a concentration $C_{A0} = 1$ mol/liter is introduced into a batch reactor where it reacts away to form product R according to stoichiometry $A \rightarrow R$. The concentration of A in the reactor is monitored at various times, as shown below:

t, min	0	100	200	300	400
C_A, mol/m^3	1000	500	333	250	200

For $C_{A0} = 500$ mol/m^3 find the conversion of reactant after 5 hours in the batch reactor.

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For $C_{A0} = 500$ mol/m^3 find the conversion of reactant after 5 hours in the batch reactor.

From the table of data

at $C_A = 500 \quad t = 100$ min

Thus

at $t = 5$ hrs $+ 100$ min $= 400$ min

$C_A = 200 \frac{mol}{m^3}$ ... or $X_A = 0.6$.

Problem 5

The rate constant of thermal decomposition of a reactant at different temperature is reported as follows

T, °C	508	427	393	356	283
k, $cm^3/mol \cdot s$	0.1059	0.003 10	0.000 588	80.9×10^{-6}	0.942×10^{-6}

The units of the rate constant tells that this is a $2^{\underline{nd}}$ order reaction

$$-r_A = kC_A^2 = k_o e^{-E/RT} C_A^2$$

Thus

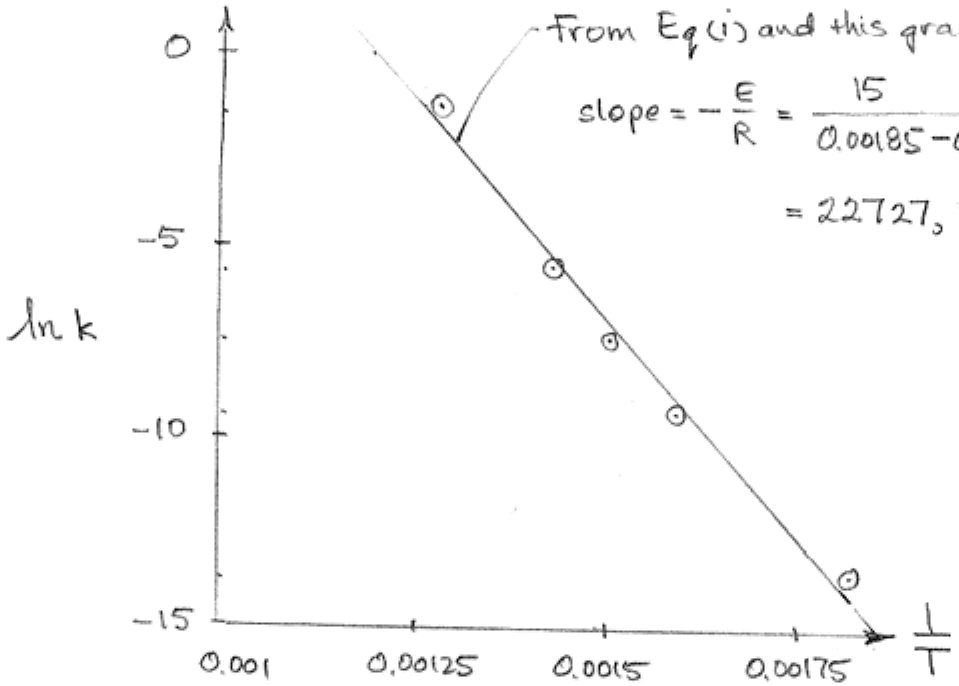
$$k = k_o e^{-E/RT}$$

or

$$\ln k = \ln k_o - \frac{E}{R}\left(\frac{1}{T}\right)$$

First let us tabulate

T, °C	T, K	1/T, K^{-1}	k	ln k
508	781	0.00128	0.1059	−1.6974
427	700	0.00143	0.0031	−5.7764
393	666	0.001502	0.000588	−7.4388
356	629	0.001590	80.9×10^{-6}	−9.4223
273	546	0.001832	0.942×10^{-6}	−13.8753



From Eq (i) and this graph

$$\text{slope} = -\frac{E}{R} = \frac{15}{0.00185 - 0.00119}$$

$$= 22727,\ K^{-1}$$

To find the value of k_o take the second data point.
From Eq (i)

$$\ln k_0 = \ln k - \frac{E}{R}\left(\frac{1}{T}\right)$$

$$= 5.7764 - 22727\left(\frac{1}{700}\right) = 38.2439$$

$$\text{or } k_o = e^{38.2439} = 4.06 \times 10^{16}$$

So for the temperature range covered in the reported data

$$-r_{HI} = 4.06 \times 10^{16}\, e^{-22727/T}\, C_A^2, \quad \text{mol/cm}^3\cdot\text{s}$$