Experiment-1

Rate Study in a Plug Flow Reactor
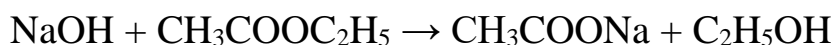
18CH10071, Anshuman Agrawal

Objectives

1. To determine the order of reaction between sodium hydroxide and ethyl acetate using a plug flow reactor.
2. To find the rate constant at a particular temperature.

Theory

Stoichiometric Equation:

$$NaOH + CH_3COOC_2H_5 \rightarrow CH_3COONa + C_2H_5OH$$

   (A)   (B)   (C)   (D)

Mole balance: $\dfrac{V_R}{F_{A_0}} = \int_0^{X_A} \dfrac{dX_A}{-r_A}$
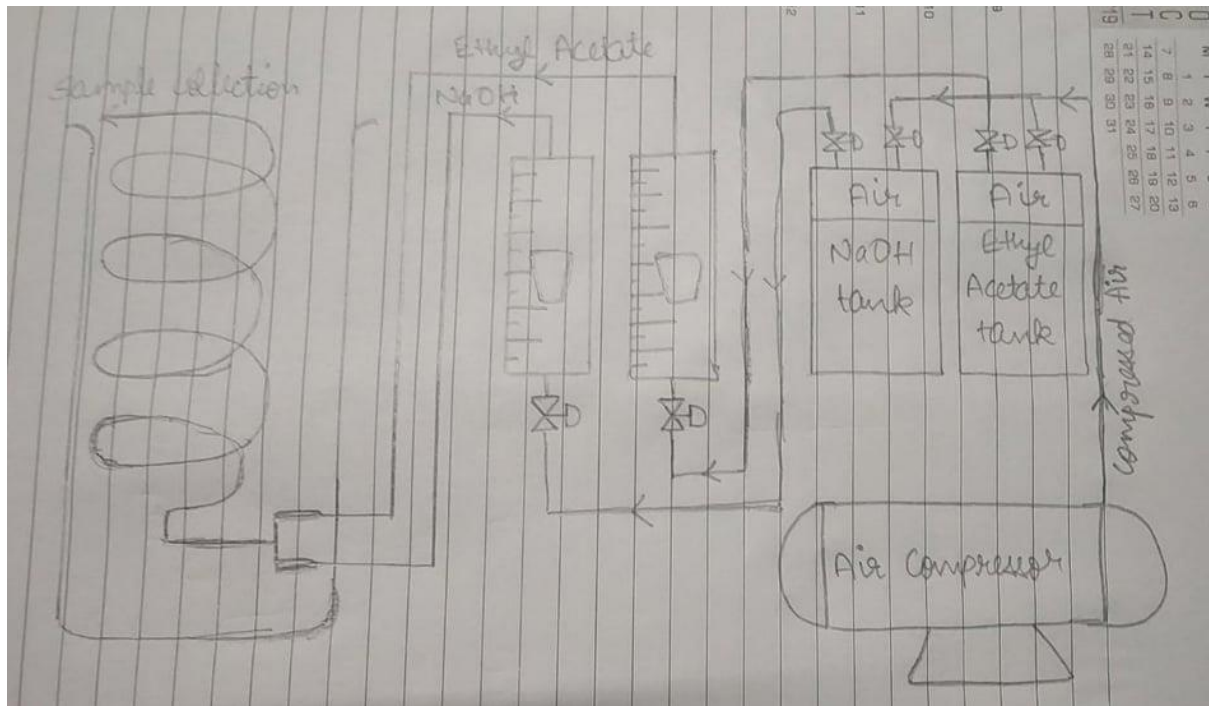
Rate Equation: $-r_A = k_2 C_{A_0}^2 (1 - X_A)(M - X_A)$

Where $M = \dfrac{C_{B_0}}{C_{A_0}}$, X_A = conversion of A, k_2 = rate constant

$$\frac{V_R}{F_{A_0}} = \frac{V_R}{v_0 C_{A_0}} = \frac{\tau}{C_{A_0}} = \frac{1}{k_2 C_{A_0}^2 (M-1)} \ln \frac{M - X_A}{M(1 - X_A)} = \frac{1}{k_2} f(X_A)$$

Where $v_0 = v_A + v_B$ and $\tau = \dfrac{V_R}{v_0}$

Schematic

Observations

Strength of Succinic Acid = N/50 = 0.02 N = 0.01 M (dibasic acid)
C_{A0} (before mixing) = 0.049 mol/ L
C_{A0} (after mixing) = 0.0245 mol/ L
C_{B0} (before mixing) = 0.1 mol/ L
C_{B0} (after mixing) = 0.05 mol/ L
Reactor volume = 0.724 L
Length of coil = 609.6 cm
Inside diameter of tube = 1.23 cm
M = 2.04

Flow Rate (LPH)	τ (sec)	C_{A0} (mol/L)	Titre Volume (ml)	X_A	Average X_A	$f(X_A)$
7.5	173.76		1.7	0.722	0.706	1280.57
			1.8	0.706		
			1.9	0.690		
10	130.32	0.0245	2	0.673	0.635	1017.12
			2.2	0.641		
			2.5	0.592		
12.5	104.26		2.5	0.592	0.587	873.01
			2.5	0.592		
			2.6	0.576		

Sample Calculations

For titre value of 1.7 ml,

$N_1 V_1 = N_2 V_2$ (meq balance for titration)

$0.02 \times 1.7 = N_2 \times 5 \Rightarrow N_2 = 0.0068$

$N_2 = M_2 = 0.0068 \text{ mol}/L$ ($\because$ NaOH is a monoacidic base)

$X_A = \dfrac{0.0245 - 0.0068}{0.0245}$

$= 0.722$

similarly for 1.8 ml and 1.9 ml, $X_A = 0.706$ and $X_A = 0.69$ respectively.

Average $X_A = \dfrac{0.69 + 0.706 + 0.722}{3}$

$= 0.706$

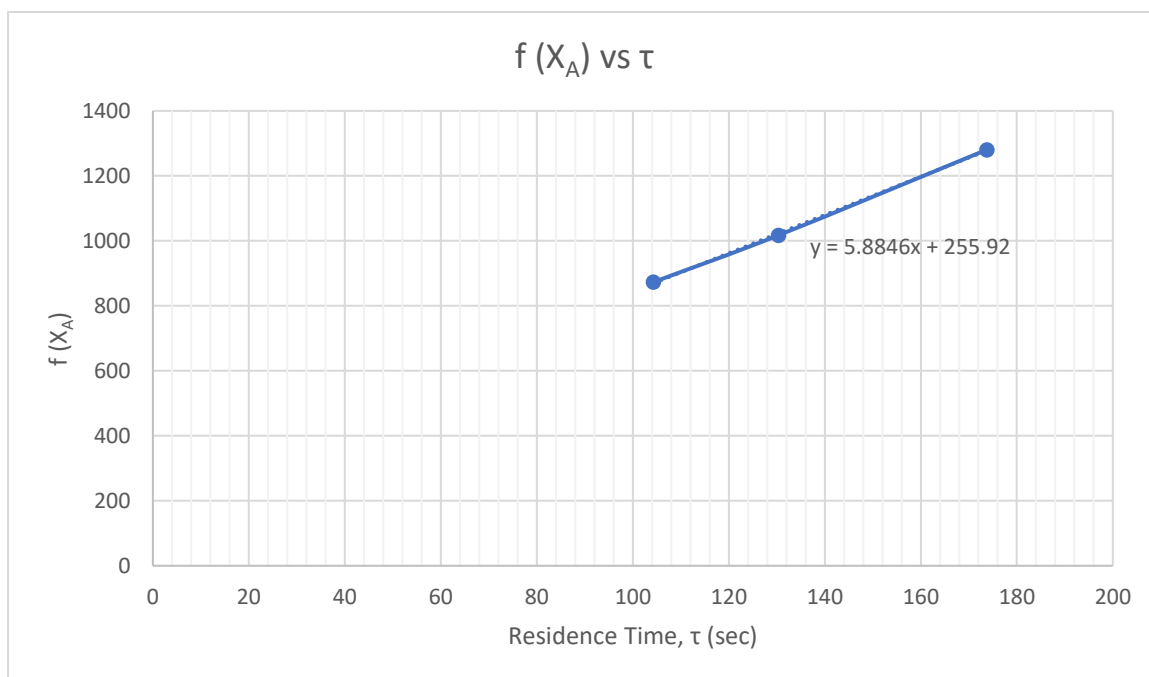$f(X_A) = \dfrac{1}{C_{A_0}^2 (M-1)} \ln\left(\dfrac{M - X_A}{M(1 - X_A)}\right)$

$f(X_A) = \dfrac{1}{0.0245^2 (1.04)} \ln\left(\dfrac{2.04 - 0.706}{2.04(1 - 0.706)}\right)$

$= 1280.57 \; l^2/\text{mol}^2$

$\tau = \dfrac{V_R}{v_0} = \dfrac{0.724}{7.5 + 7.5} \times 3600 = 173.76 \text{ sec.}$

Plot

f (X_A) vs τ

y = 5.8846x + 255.92

Results

Slope of above plot = 5.8846 $l^2\,mol^{-2}\,s^{-1}$
Rate constant = slope $\times$ C_{A0} = 5.8846 $\times$ 0.0245 = 0.144 $l\,mol^{-1}\,s^{-1}$
Therefore, the rate constant of given reaction at existing temperature conditions is **0.144 l mol^{-1} s^{-1}**

Discussion
- The conversion is seen to decrease with increasing flow rate which seems logical given the residence time is decreasing.
- Rotameters are one possible source of error because the marker inside never stays in full equilibrium state therefore, there is always a very small error adding to the system.
- During titration, the final solution is not exactly neutral since phenolphthalein changes colour at pH > 7.
- Care must be taken that the phenolphthalein is not added in excess while titrating to the mixture.
- During titration, another possible error can occur due to parallax in taking the titre value if the meniscus is not observed carefully.

Conclusion

With this assumed 2nd order reaction taking place in a PFR, we can easily observe the desired results and trends between all relevant values. The rate constant value obtained for the reaction occurring in the PFR is a reasonable value considering the existing temperature conditions.