The University of Jordan

School of Engineering

Department of Chemical Engineering

Chemical Engineering Laboratory (4) (0905562)

Section no. (1)

Experiment no. (4)

Tubular Reactor

Short Report

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ABSTRACT

The experiment involved a tubular reactor, a cylindrical reactor configuration that enables continuous flow of reactants through its length. The aim was to analyze the effects of operational parameters on conversion. In the first set of runs, where the flow rate decreased and the residence time was low, the conversions were 0.64, 0.61, and 0.51, respectively, at a constant temperature. In the subsequent runs, with a constant flow rate but varying temperatures, the conversions were 0.61, 0.66, and 0.69, respectively. The increase in conversion with higher temperatures indicated an elevated reaction rate due to the temperature-dependent rate constant. Additionally, the rate of the reaction was obtained graphically, yielding a rate constant (k_0) value of 420836.6 L/mol.s. Furthermore, the activation energy (E_a) was determined to be 36180.03 J/mol. These results emphasized the influence of both residence time and temperature on conversion within the tubular reactor, and the significance of the activation energy in controlling the reaction rate.

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RESULTS

A. Determination of the rate constant and the effect of changing the inlet flowrates on the conversion

Table 1: Experimental Data

Run	C_A (mol/L)	C_B (mol/L)	F_A (ml/min)	F_B (ml/min)	F_A (L/s)	F_B (L/s)	C_{A0} (mol/L)	C_{B0} (mol/L)	C_{A1} (mol/L)	T (°C)	T (°K)
1	0.06	0.06	40	40	0.00067	0.00067	0.03	0.03	0.01091	22.8	295.95
2	0.06	0.06	50	50	0.00083	0.00083	0.03	0.03	0.01163	22.8	295.95
3	0.06	0.06	60	60	0.001	0.001	0.03	0.03	0.01471	22.8	295.95

Table 2: Calculated Data

Run	t_R (s)	X_a	$X_a/(1-X_a)$	k (L/mol.s)
1	349.5	0.64	1.75	0.17
2	279.6	0.61	1.58	0.19
3	233	0.51	1.04	0.15
K_{avg} (L/mol.s)				0.17

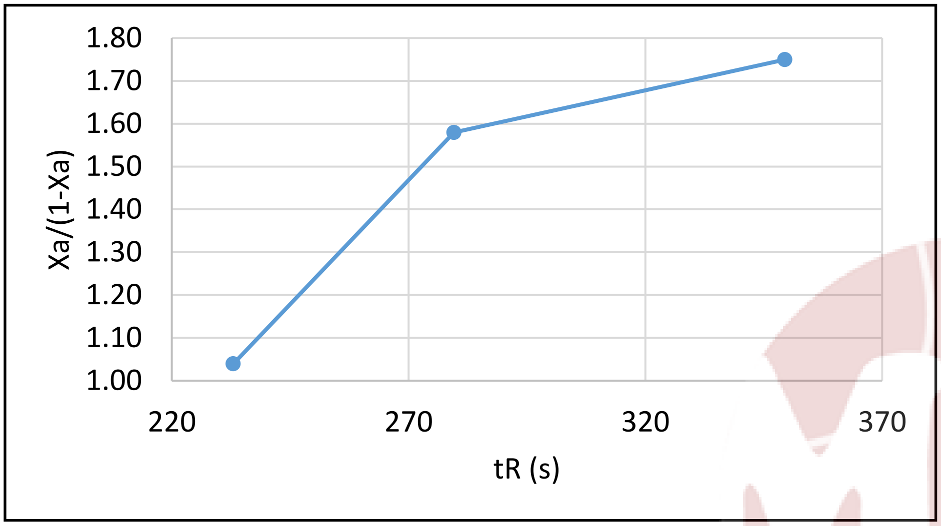


Figure 1: Residence Time vs. (Xa/1-Xa)

B. Demonstration of the rate constant dependance on the reaction temperature

Table 3: Experimental Data

Run	C_A (mol/L)	C_B (mol/L)	F_A (ml/min)	F_B (ml/min)	F_A (L/s)	F_B (L/s)	C_{A0} (mol/L)	C_{B0} (mol/L)	C_{A1} (mol/L)	T (ºC)	T (ºK)
1	0.06	0.06	50	50	0.00083	0.00083	0.03	0.03	0.01163	22.8	295.95
2	0.06	0.06	50	50	0.00083	0.00083	0.03	0.03	0.0103	32	305.15
3	0.06	0.06	50	50	0.00083	0.00083	0.03	0.03	0.00617	42	315.15

Table 4: Calculated Data

Run	t_R (s)	X_a	$X_a/(1-X_a)$	k (L/mol.s)	ln(k)	1/T(ºK)
1	279.6	0.61	1.58	0.19	-1.67	0.0034
2	279.6	0.66	1.91	0.23	-1.48	0.0033
3	279.6	0.79	3.86	0.46	-0.78	0.0032

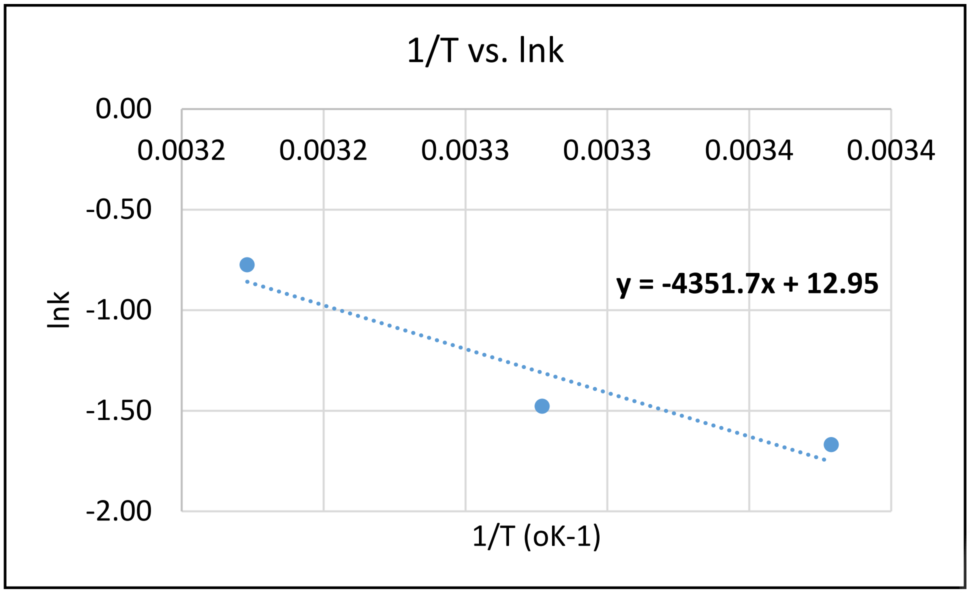


Figure 2: 1/T vs. lnk

Table 5: Reaction Rate Constant as A Function of Temperature

E (J/ mol)	k_0 (L/mol.s)
36180.0338	420836.6363
$k = 420836.6e^{\frac{36180}{RT}}$	

DISCUSSION

At a Constant temperature

As shown in table (2), the conversion of $NaOH$ was found at different flow rates. The runs were investigated at equal flow rates of reactants. Three different feed flow rates

($0.00067\ L/s, 0.00083\ L/s\ and\ 0.001\ L/s$) and the experiments were conducted at a constant temperature of $295.4\ K$.

Conversion reaches a value of $X = 0.64$ at a flow rate of $0.00067\ L/s$ in comparison with a value of $X = 0.51$ at a flow rate of $0.001\ L/s$ so the conversion of $NaOH$ decrease with increase the flow rate there is an inverse relation. Residence time decreases with increased reactant flow rate, we can conclude that the higher the flow rate, the lower residence time and lower conversion. The conversion is referred to how many moles of $NaOH$ are reacted to form a product over a time. Residence times refer to the time taken needed to process one volume of the reactor fluid at the entrance condition.

At a Constant flow rate

As shown figure (2), When the temperature increases, the fraction of molecules that have kinetic energies more than the activation energy of the reaction increases ($36180\ J\ /\ mol$)

Therefore, as increases the reaction temperature, the rate of the reaction constantly increases and the conversion increases.

CONCLUSION AND RECOMMENDATIONS

- Tubular reactors operate in a continuous flow mode to maintain a steady-state operation, meaning that reactants are continuously fed into the reactor, and the products are continuously removed.
- The residence time of the reactants in the reactor controlled by adjusting the flow rate. To ensure that the reaction reaches completion.
- Tubular reactors often provide better mixing and uniformity of reaction conditions along the length of the tube. This contributes to a more consistent and predictable reaction environment.
- At a constant temperature, lower flow rates resulted in higher NaOH conversion. While higher flow rates, led to decreased conversion.
- Under constant flow rates, an increase in temperature resulted in a higher fraction of molecules surpassing the activation energy. This led to an increased rate of reaction and, consequently, higher conversion. Temperature is a key factor influencing reaction kinetics.
- The frequency factor is temperature dependent as it is related to molecular collisions.
- It is recommended to increase the range of temperatures and flow rates to get a more comprehensive understanding of the reaction kinetics.
- It is recommended to ensure that the reaction reaches equilibrium and steady state between reactants, especially in continuous flow operations.

REFERENCES

1. Atkins, P. W., Trapp, C. A., & Julio De Paula. (2010). Physical chemistry [Hauptbd.]. Oxford Oxford Univ. Press.

2. Chemical Engineering Laboratory (4) Manual Sheet. (2022). 1st ed. University of Jordan School of Engineering Department of Chemical Engineering.

3. H Scott Fogler (1999). Elements of chemical reaction engineering. Upper Saddle River, Nj: Prentice-Hall.

APPENDICES

Derivation of Equations:

→In this experiment, the following second order reaction was studied:

$$-r_A = k.C_A C_B$$

$$-r_A = k.C_A^2 \quad , \quad where \quad C_A = C_B$$

OR

$$-\frac{dC_A}{dt} = k.C_A^2 \quad \rightarrow \quad -C_{A0}\frac{d(1-x)}{dt} = k.C_{A0}^2.(1-x)^2$$

$$\frac{dx}{dt} = k.C_{A0}.(1-x)^2$$

$$\int_0^x \frac{dx}{(1-x)^2} = \int_0^t k.C_{A0}.dt$$

$$Integration\ by\ substitution: \quad z = 1-x, \quad dz = -dx$$

$$\int \frac{-dz}{z^2} = \frac{1}{z} = \frac{1}{1-x}$$

$$\frac{1}{1-x} - 1 = k.C_{A0}.t_R$$

$$\frac{x}{1-x} = k.C_{A0}.t_R$$

$$\boxed{k = \frac{x}{(1-x).C_{A0}.t_R}}$$

$$-\frac{dC_A}{dt} = k.C_A^2$$

$$-\int_{C_{A0}}^{C_A} \frac{dC_A}{C_A^2} = \int_0^t k.dt$$

$$\frac{1}{C_A} - \frac{1}{C_{A0}} = kt \quad ,t = \frac{V}{F_A + F_B}$$

$$\boxed{k = \frac{(C_{A0} - C_A).(F_A + F_B)}{C_A C_{A0} V}}$$

Sample of calculations for first run in rate constant determination:

$$F_A = F_B = 40\,\frac{ml}{min}.\frac{1\ L/s}{6 * 10^4\ ml/min} = 6.7 * 10^{-4}\,\frac{L}{s}$$

$$T = 22.8\ ℃ + 273.15 = 295.95\ °K$$

- Initial Concentrations

$$C_{A0} = \frac{F_A}{F_A + F_B}.C_A = \frac{6.7 * 10^{-4}}{6.7 * 10^{-4} + 6.7 * 10^{-4}} * 0.06 = 0.03\ \frac{mol}{L}$$

$$C_{B0} = \frac{F_B}{F_A + F_B}.C_B = \frac{6.7 * 10^{-4}}{6.7 * 10^{-4} + 6.7 * 10^{-4}} * 0.06 = 0.03\ \frac{mol}{L}$$

- Residence Time

$$t_R = \frac{V}{F_A + F_B} = \frac{0.466}{6.7 * 10^{-4} + 6.7 * 10^{-4}} = 349.5\ s$$

- Conversion

$$x_a = \frac{C_{A0} - C_{A1}}{C_{A0}} = \frac{0.03 - 0.01091}{0.03} = 0.64$$

- Rate Constant

$$k = \frac{(C_{A0} - C_{A1}).(F_A + F_B)}{C_A C_{A0} V} = \frac{(0.03 - 0.01091) * (6.7 * 10^{-4} + 6.7 * 10^{-4})}{0.03 * 0.01091 * 0.466} = 0.167\ \frac{L}{mol.s}$$

Sample of calculations for first run in determining the rate constant dependance on the reaction temperature

- Initial Concentrations

$$C_{A0} = \frac{F_A}{F_A + F_B}.C_A = \frac{8.3 * 10^{-4}}{8.3 * 10^{-4} + 8.3 * 10^{-4}} * 0.06 = 0.03\ \frac{mol}{L}$$

$$C_{B0} = \frac{F_B}{F_A + F_B}.C_B = \frac{8.3 * 10^{-4}}{8.3 * 10^{-4} + 8.3 * 10^{-4}} * 0.06 = 0.03\ \frac{mol}{L}$$

- Residence Time

$$t_R = \frac{V}{F_A + F_B} = \frac{0.466}{8.3 * 10^{-4} + 8.3 * 10^{-4}} = 279.6\ s$$

- Conversion

$$x_a = \frac{C_{A0} - C_{A1}}{C_{A0}} = \frac{0.03 - 0.01163}{0.03} = 0.61$$

- Rate Constant

$$k = \frac{x}{(1-x).C_{A0}.t_R} = \frac{0.61}{(1-0.61) * 0.03 * 279.6} = 0.19\ \frac{L}{mol.s}$$

- Reaction rate constant as a function of temperature

$$\ln k = \ln 0.19 = -1.67$$

$$\ln k = \ln k_0 - \frac{E}{RT}$$

$$\frac{1}{T} = \frac{1}{295.95} = 0.0034\ °K^{-1}$$

→By plotting 1/T versus lnk and linearizing the data, the following equation was obtained:

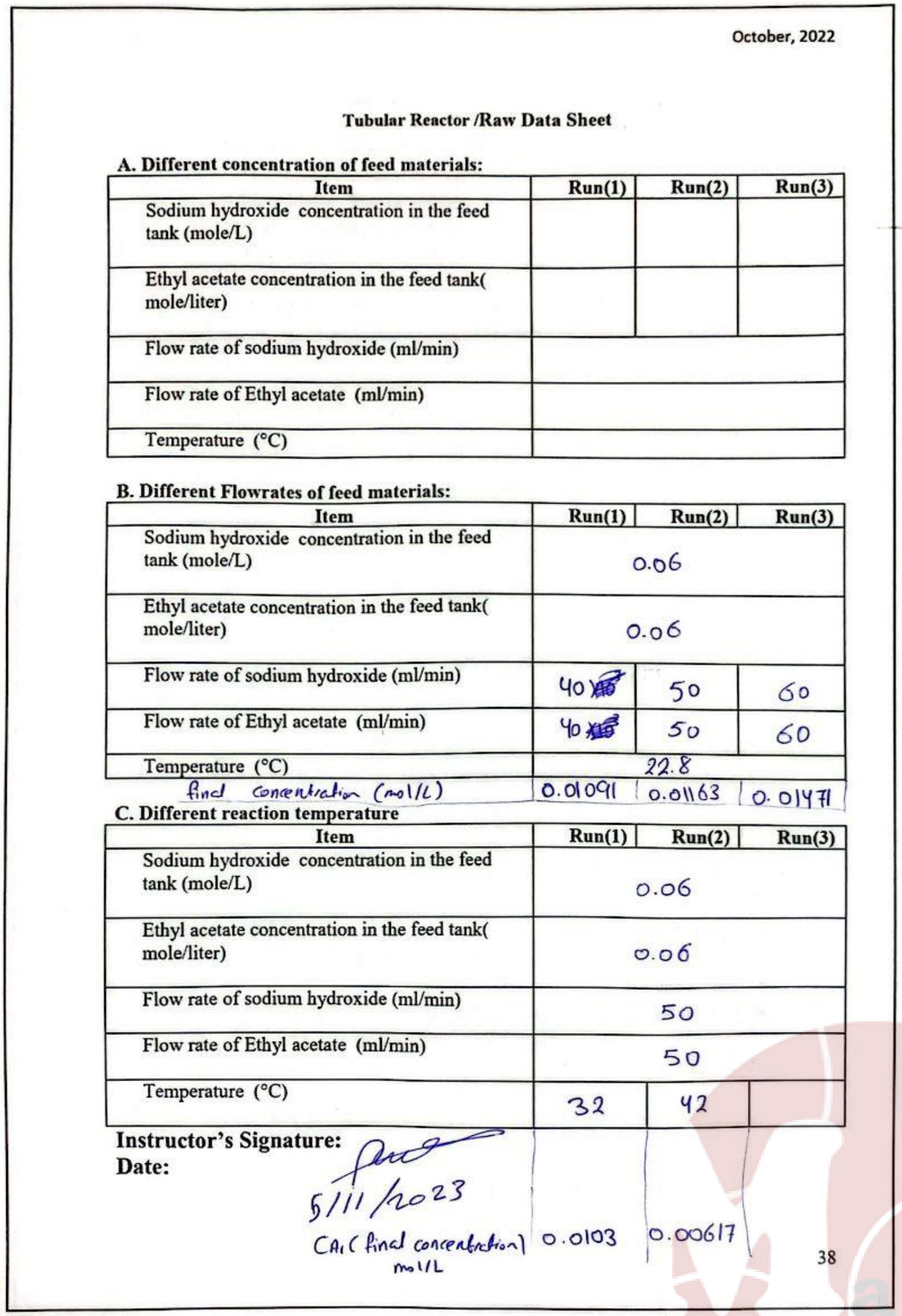
y = -4351.7x + 12.95

$$E = -R.Slope = -8.314 * -4351.7 = 36180\ J/mol$$

$$k_0 = e^{intercept} = e^{12.95} = 420836.64\ \frac{L}{mol.s}$$

$$\boxed{k(T) = 420836.6e^{\frac{36180}{RT}}}$$

Data Sheet



October, 2022

Tubular Reactor /Raw Data Sheet

A. Different concentration of feed materials:

Item	Run(1)	Run(2)	Run(3)
Sodium hydroxide concentration in the feed tank (mole/L)			
Ethyl acetate concentration in the feed tank(mole/liter)			
Flow rate of sodium hydroxide (ml/min)			
Flow rate of Ethyl acetate (ml/min)			
Temperature (°C)			

B. Different Flowrates of feed materials:

Item	Run(1)	Run(2)	Run(3)
Sodium hydroxide concentration in the feed tank (mole/L)	0.06		
Ethyl acetate concentration in the feed tank(mole/liter)	0.06		
Flow rate of sodium hydroxide (ml/min)	40	50	60
Flow rate of Ethyl acetate (ml/min)	40	50	60
Temperature (°C)	22.8		
final concentration (mol/L)	0.01091	0.01163	0.01471

C. Different reaction temperature

Item	Run(1)	Run(2)	Run(3)
Sodium hydroxide concentration in the feed tank (mole/L)	0.06		
Ethyl acetate concentration in the feed tank(mole/liter)	0.06		
Flow rate of sodium hydroxide (ml/min)	50		
Flow rate of Ethyl acetate (ml/min)	50		
Temperature (°C)	32	42	
CA₁ (final concentration) mol/L	0.0103	0.00617	

Instructor's Signature:

Date: 5/11/2023