CHE 392 CEHEMICAL ENGINEERING LABORATORY I

Experiment # : 4 a
DETERMINATION OF REACTION RATE EXPRESSION

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PURPOSE

- Development of reaction rate expression by batch reactor data

PRELIMINARY STUDY

1. Describe the reaction rate expression.
2. Describe reactor types and operating principles.
3. Write the material balance for a batch reactor.
4. In batch reactors, data analysis is done according to which methods?
5. What is the unit of reaction rate constant for second order kinetic?

6. By using the integral method for the second order reaction system, improve the expression of concentration change with reaction time.
7. In the reaction system where the second order reaction kinetics are valid, if one of the reagents is diluted initially, how is the concentration time relationship? How does the reaction rate constant change?
8. As known, saponification reaction is a very fast reaction. Explain how to determine the concentration by measuring the conductance.

The parameters required to improve the reaction rate expression ***?***

* initial concentrations?
* solution volume?
* temperature ?
* stirring rate of solution?
* total duration of the experiment?

Why is determination of the velocity expression in terms of reaction kinetics important?

The reaction rate enables that :

the concentration values of one or more reagents or products in a reactor vessel are known as a function of time,

the determination of the numerical value of the reaction rate constant.

The reaction chosen for this work is the saponification of ethyl acetate with sodium hydroxide.

$$\mathbf{NaOH + EtOAc \rightarrow NaOAc + EtOH}$$

It is known that the saponification reaction corresponds to a second order rate equilibrium.

$$- r_{NaOH} = - r_{EtOAc} = k\ C_{NaOH}\ C_{EtOAc}$$

$$-r_A = -\frac{dC_A}{dt} = -\frac{dC_B}{dt} = kC_A C_B$$

A: NaOH

B: EtOAc.

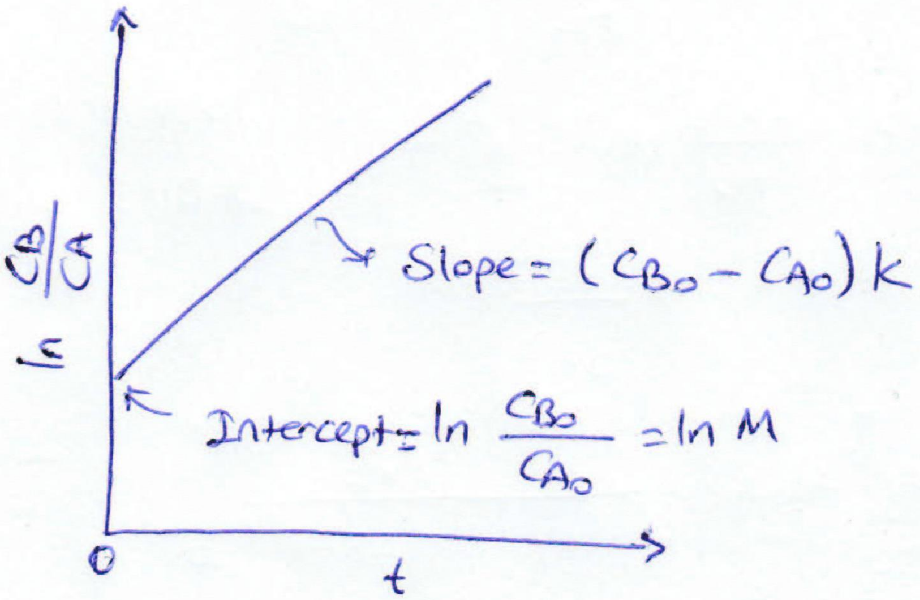
$$-r_A = C_{A0}\frac{dX_A}{dt} = k(C_{A0} - C_{A0}X_A)(C_{B0} - C_{A0}X_A)$$

$$M = \frac{C_{B0}}{C_{A0}} \qquad -r_A = C_{A0}\frac{dX_A}{dt} = kC_{A0}^2(1-X_A)(M-X_A)$$

$$\int_0^{X_A} \frac{dX_A}{(1-X_A)(M-X_A)} = C_{A0}k\int_0^t dt$$

$$\ln\frac{1-X_B}{1-X_A} = \ln\frac{M-X_A}{M(1-X_A)} = \ln\frac{C_B C_{A0}}{C_{B0} C_A} = \ln\frac{C_B}{MC_A}$$

$$= C_{A0}(M-1)kt = (C_{B0} - C_{A0})kt \qquad M \neq 1$$



$A + B \rightarrow R$. $C_{A0} \neq C_{B0}$. 2nd order rxn.

Arrhenius equation

$$\ln k = \ln A - \frac{E_a}{RT}$$

$\ln k$ versus $\frac{1}{T}$ graph is drawn.

Slope of the line: $-\frac{E_a}{R}$

Intercept: $\ln A$

A: Frequency factor.

E_a: Activation energy.

Experimental Part

Chemical Solutions

- 0.1 M NaOH
- 0.1 M EtOAc
- 0.1 M NaOAc

Laboratory equipments

- Conductivity meter
- Magnetic stirrer
- 250 mL erlen, 50 mL ve 250 mL graduated cylinders
- Water bath, ice
- Thermometer
- Kronometer

Experimental Procedure

After 125 mL of NaOH and EtOAc solutions having the desired C_{A0} and C_{B0} values are prepared, place them in the seperate erlen meyers.

Add the probe of the conductivity meter into the NaOH solution at the desired temperature on the magnetic stirrer. While pour EtOAc solution at the same temperature into the NaOH solution, immediately record the change in the conductivity value of the total solution during reaction time.

For temperature adjustments of the solutions, you can use a heater of magnetic stirrer and ice bath.

Experimental Data

	G_0 (mS/cm)	G_{100} (mS/cm)
17°C	11.41	3.75
22°C	11.20	3.75
32°C	10.85	3.75

Lineer changes in conductivity values will be assumed during exp. time, total conversion

$$X = \frac{C_{NaOH,0} - C_{NaOH}}{C_{NaOH,0}} \cdot 100\,\%$$

$C_{A0} = 0{,}05146$ M

$C_{B0} = 0{,}04115$ M

$$X_{NaOH} = 100\,\% \left(1 - \frac{G - G_{100}}{G_0 - G_{100}}\right)$$

$$X = \frac{G_0 - G}{G_0 - G_{100}}$$

G: Conductivity value of solution at t

G_0: " " when 0% NaOH conversion

G_{100}: " when 100% "

100 % conversion will be assumed in 20 minutes.

EVALUATION OF DATA

1. Create the concentration time change for each experiment.
2. Determine the reaction order using the data.
3. Create the Arrhenius relationship for the reaction.
4. Create the generally defined reaction rate expression by means of the calculated rate parameters.

I expect you to prepare your report by paying attention to the report writing rules and send it within 15 days.

If you have any questions, you can ask by sending a message.

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