Chemical Technology Lab. I

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HOMOGENEOUS BATCH REACTOR

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1. HOMOGENEOUS BATCH REACTOR

1.1 Objective

To determine the order and value of the rate constant for the liquid reaction of caustic soda and ethyl acetate in a batch reactor:

$$\mathbf{NaOH + CH_3COOC_2H_5 \rightarrow C_2H_5OH + CH_3COONa}$$

1.2 Introduction

A batch reactor may be described as a vessel in which chemicals are placed to react. Batch reactors are normally used in small-scale laboratory set-ups to study the kinetics of chemical reactions.

To determine the order and constant of a chemical reaction, the variation of a property of the reaction mixture is observed as the reaction progresses. Data collected usually consist of changes in variables such as concentration of a component, total volume of the system or a physical property like electrical conductivity or refractive index. The data are then analyzed using pertinent equations to find desired kinetic parameters.

1.3 Theory

For any given reaction in a constant volume system, the rate of the reaction can be represented by:

$$-r_A = kf(C_A) = -\frac{dC_A}{dt} \qquad (1.1)$$

Where r_A is the rate of disappearance of reactant A among the reacting species. Equation (1) can be rearranged to give:

$$-\frac{dC_A}{f(C_A)} = kdt \qquad (1.2)$$

Integrating equation (1.2) analytically yields

$$-\int_{C_{A_0}}^{C_{A_f}} \frac{dC_A}{f(C_A)} = k\int_0^t dt = kt \qquad (1.3)$$

By postulating various forms for f (C_A) in equation (1.3) and correlating the resulting equation with the experimental data, the rate constant k, and order of the reaction can be determined.

1.4 Procedure

1. In the reactor, mix 1.0 liter of the 0.1M Caustic Soda (NaOH) solution with 1.0 liter of the 0.1M ethyl acetate solution at an arbitrary time (t = 0) at room temperature. Start the stirrer immediately at an intermediate speed to avoid splashing.

2. After a certain time, interval, using a flask or graduated cylinder withdraw a sample of known size (e.g., 25 ml) from the opening in the base of the reactor, and immediately quench this sample with an excess of 0.05M Hydrochloric Acid (HCl) (e.g. 25 ml).

3. Backtitrate the quenched sample with 0.05M NaOH solution. The required amount of 0.05M NaOH should be recorded since this will enable you to determine the concentration of NaOH in the reactor at the time you withdrew the sample.

4. Note that a drop or two of phenolphthalein should be added to the quenched sample to detect the end point (i.e., stable new color) before you backtitrate. Stirring the flask is also required during backtitration.

5. Repeat steps (2) and (3) every 5-10 minutes (and record the time for each new sample) until the amount of NaOH needed in the backtitration is nearly equal to the amount of the quenching acid.

Note 1

Make sure to withdraw and analyze at least five samples of the reactor contents during the first 15 minutes of the reaction. To accomplish this, it is recommended that you prepare known quantities (25 ml) of the acid in different flasks before the start of the reaction. You can then withdraw the samples from the reactor quench, backtitrate, etc.

1.5 Report Requirement

1. Calculate the number of moles of unreacted NaOH in each sample withdrawn.

2. Calculate the concentration of unreacted NaOH (mol/lit).

3. Apply the integral method of analysis to determine the reaction order and rate constant of the reaction. This should involve assuming an expression for the reaction rate, substituting it into equation 3, integrating, and then plotting.
4. Calculate the half-life of NaOH.
5. Determine the fractional conversion of NaOH at the end of the reaction.
6. Find both the order and rate constant of the reaction from literature compare between the theoretical and experimental values and give reasons for the deviations.

Note 2

You must give the exact reference i.e author, title, and page number of the book from which values were obtained.

1.6 References

1. Levenspiel, O., "*Chemical Reaction Engineering*", 2nd ed., Wiley and sons, N.Y., p.41 (1977).
2. Smith J.M., "*Chemical Engineering Kinetics*", 3rd ed., McGraw-Hill Book Comp. N.Y., p.37 (1981).