Experimental Determination of Kinetic Rate Constants Using Batch and CSTR Reactors

CHE-431 – UNIT OPERATIONS LAB I

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Experimental Determination of Kinetic Rate Constants

Using Batch and CSTR Reactors

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In this experiment, the use of both a batch reactor and a CSTR will be demonstrated to generate data for the determination of kinetic parameters.

The reaction

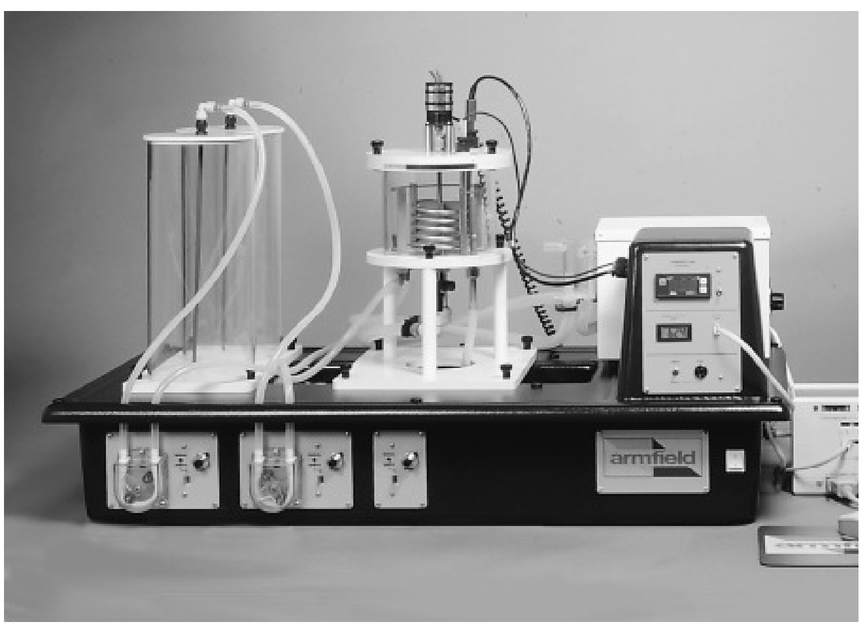
The reaction selected in this experiment is the saponification of ethyl acetate. This reaction is elementary and second-order. The reaction equation is

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

$$A \quad + \quad B \quad \rightarrow \quad C \quad + \quad D$$

The apparatus

The apparatus is the Armfield continuous stirred tank reactor which is designed to study the kinetics of a chemical reaction in this type of reactor (as well as the special case when it is run as a batch reactor). It can conveniently be used to study the effects of varying the process conditions such as reaction temperature, reactor volume, stirring rate, feed rate etc. on reaction kinetics.



CEX fitted with CEM MkII continuous stirred tank reactor

General Procedure

The reactor volume can be varied by adjusting the height of the internal standpipe. The actual volume can be checked by filling the reactor with water to the overflow then draining the reactor contents into a measuring cylinder.

For the CSTR experiment, the feed pumps should be calibrated. This can be achieved by pumping water from the reagent tanks to a measuring cylinder over a time period for a range of pump speeds. A calibration graph for each pump of % speed vs. flow rate (ml/min) can then be drawn.

The conductivity of the reacting solution in the reactor changes with the degree of conversion and this provides a convenient method for monitoring the progress of the reaction either manually or by computer.

In this experiment, the manual procedure is used. Thus, the conductivity can be recorded manually at suitable time intervals (half a minute or so) by reading the value directly from the conductivity meter in the console.

The reaction temperature can be varied and maintained using the special heater available in accordance with the instructions given in the Armfield manual which is available on this company's website or can be accessed by clicking Armfield manual as given in the website www.the-seventh-dimension.com.

Theory

For a bimolecular second order reaction, the rate equation is:

$$r = k\ C_A C_B$$

The stoichiometric equations in terms of fractional conversion X are:-

$$C_A = C_{Ao} - C_{Ao}X_A = C_{Ao}(1 - X_A)$$
$$C_B = C_{Bo} - C_{Bo}X_B$$

But when ,

$$C_{Ao} = C_{Bo} \quad \text{and} \quad C_{Ao}X_A = C_{Bo}X_B$$

Then, C_B is also equal to $C_{Ao}(1 - X_A)$ and the rate equation becomes:-

$$r = kC_{Ao}^2(1 - X_A)^2$$

A) Batch Reactor

For a constant volume isothermal batch reactor, the component mass balance equation is:

$$\frac{1}{V}\frac{dN_A}{dt} = \frac{dC_A}{dt} = (r_A)_{app} = -r \qquad (1)$$

Combining the above equations, equation (1) becomes:-

$$\frac{dC_A}{dt} = -kC_{Ao}{}^2(1-X_A)^2$$

But

$$\frac{dC_A}{dt} = -C_{Ao}\frac{dX_A}{dt}$$

Then the result is:-

$$\frac{dX_A}{dt} - kC_{Ao}(1-X_A)^2$$

Integration will yield:

$$\frac{X_A}{1-X_A} = k\ t\ C_{Ao} \qquad (2)$$

Equation (2) can be easily used to determine the value of *k*.

B) CSTR

For an isothermal steady state CSTR, the component mass balance equation is:

$$F_{Ao} - F_A + V\,(r_A)_{app} = 0$$

Since for a flow reactor $C_A = F_A / Q$ and since Q is constant (constant volume system), then this equation becomes:-

$$QC_{Ao} - QC_A + V\,(-r) = 0$$

Substituting for r , and using the previously mentioned stoichiometric equations, the following equation can be obtained:-

$$\frac{V}{Q} = \frac{X_A}{kC_{Ao}(1-X_A)^2} \qquad (3)$$

Equation (3) can then be used to determine the value of *k*.

Conductivity as a measure of conversion

The measurements of conductivity Λ are related to the conductivity of a sodium hydroxide (A) and sodium acetate (C) solution as follows:-

$$\Lambda = \Lambda_A + \Lambda_C$$

where :

$$\Lambda_A = 0.195\,[1 + 0.01184(T - 294)]C_A \qquad \text{For T > 294K}$$

$$\Lambda_C = 0.07\,[1 + 0.0284(T - 294)]C_C \qquad \text{For T > 294K}$$

Using the stoichiometric equations given previously to eliminate C_A and C_C in terms of X_A, then an equation for X_A in terms of Λ, C_{Ao}, and T can be easily obtained (eq. 4). You need to derive such an equation in the simplest possible form and use it. Use of the equations in the Armfield Manual to calculate conversion is not acceptable.

Report

The report should conform to the outline provided to you by the Lab instructors. Your grade will depend to a great extent on following that outline closely. In addition to that, the following should be included in the report:-

1) Detailed derivation of equations (2) and (3) as well as eq.(4) mentioned previously for calculating X_A.

2) Determination of the rate constant of the reaction from the data obtained using the batch reactor and the CSTR. Sample calculations are required.

3) Comparison of results obtained from both reactors, as well as comparison with the experimental data reported in the literature for similar conditions.

4) Comments on the differences in the results obtained and discussion of the results and the quality of the data and experimental procedures (difficulties and uncertainties).

References

1. Levenspiel, O., Chemical Reaction Engineering, John Wiley & Sons, Toronto, Ed. 2, 1972, p. 283-90.

2. Armfield manual.