CHAPTER

FIVE

REACTION ENGINEERING

5.1. Determination of Kinetic Parameters of the Saponification Reaction in a PFR

5.2. Determination of Kinetic Parameters of the Saponification Reaction in a CSTR

5.3. Experimental and Numerical Determination of Kinetic Parameters of the Saponification Reaction in a Series of CSTRs

5.1. DETERMINATION OF KINETIC PARAMETERS OF THE SAPONIFICATION REACTION IN A PFR

Keywords: *Tubular reactor, plug flow reactor, saponification, integral method, differential method.*

Before the experiment: *See your TA before the experiment. Read the booklet carefully. Be aware of the safety issues. Make sure to do all solution preparation calculations before you come to lab.*

Ethyl Acetate Mol wt.: 88.10, Density: 0.898 g/cm^3 (liquid)
Sodium Hydroxide Mol wt.: 40.00 (pellet)

5.1.1. Aim

To study the saponification of ethyl acetate in a plug-flow reactor and to determine the kinetic parameters using two different evaluation methods.

5.1.2. Theory

5.1.2.1. Plug Flow Reactor

In a tubular reactor, the feed enters at one end of a cylindrical tube and the product stream leaves at the other end. The long tube and the lack of stirring prevent complete mixing of the fluid in the tube. Hence the properties of the flowing stream will vary from one point to another, namely in both radial and axial directions.

In the ideal tubular reactor, which is called the “plug flow” reactor, specific assumptions are made about the extent of mixing:

1. no mixing in the axial direction, i.e., the direction of flow
2. complete mixing in the radial direction
3. uniform velocity profile across the radius.

The absence of longitudinal mixing is what defines this type of reactor [1]. The validity of the assumptions will depend on the geometry of the reactor and the flow conditions. Deviations, which are frequent but not always important, are of two kinds:

1. mixing in longitudinal direction due to vortices and turbulence
2. incomplete mixing in radial direction in laminar flow conditions

For a time element Δt and a volume element ΔV at steady state, the mass balance for species 'i' is given by Eq. 5.1.1

$$v\, C_A \big|_V \Delta t - v\, C_A \big|_{V+\Delta V} \Delta t - r_A \Delta V \Delta t = 0 \qquad (5.1.1)$$

where

v : total volumetric flow rate, L/s

C_A : concentration of reactant A, mol/L

r_A : rate of disappearance of reactant A, mol/Ls

Dividing Eq. 5.1.1 by ΔV and Δt results in Eq. 5.1.2

$$\frac{v\, C_A|_V - v\, C_A|_{V+\Delta V}}{\Delta V} = -\frac{r_A}{v} \qquad (5.1.2)$$

and taking limit as ΔV → 0 gives Eq. 5.1.3.

$$\frac{dC_A}{dV} = \frac{r_A}{v} \qquad (5.1.3)$$

Eq. 5.1.4 is the relationship between concentration and size of reactor for the plug flow reactor. Here rate is a variable, but varies with longitudinal position (volume in the reactor, rather than with time) [2].

$$\frac{dV}{v} = \frac{dC_A}{r_A} \qquad (5.1.4)$$

If the equation 5.1.4 is integrated with following boundary conditions,

At the entrance: $V = 0$

$C_A = C_{A0}$ (inlet concentration of reactant A)

At the exit: $V = V_R$ (total reactor volume)

$C_A = C_A$ (exit conversion)

$$\int_0^{V_R} \frac{dV}{v} = \int_{C_{AO}}^{C_A} \frac{dC_A}{r_A} \tag{5.1.5}$$

With the elementary reaction assumption, reaction rate equation can be simplified as in Eq. 5.1.6. where C_B is concentration of reactant B and θ_B is the ratio of inlet concentrations of reactant B and A (C_{B0}/C_{A0})

$$-r_A = kC_AC_B$$

$$C_A = C_{A0}(1-X);\ \ C_B = C_{A0}(\theta_B - X) \tag{5.1.6}$$

Combining equations 5.1.7 and 5.1.8, the following expression (Eq. 5.1.7) is obtained.

$$\int_0^{V_R} \frac{dV}{v} = -\int_{C_{AO}}^{C_A} \frac{dC_A}{kC_AC_B} \tag{5.1.7}$$

It can be written in terms of conversion as Eq. 5.1.8 [3].

$$\int_0^{V_R} \frac{dV}{v} = -\int_{C_{AO}}^{C_A} \frac{dC_A}{kC_{A0}{}^2(1-X)(\theta_B - X)} \tag{5.1.8}$$

5.1.2.2. Saponification Reaction

$$\text{Sodium Hydroxide} + \text{Ethyl Acetate} \rightarrow \text{Sodium Acetate} + \text{Ethanol}$$

The reaction is 2nd order elementary within the range of 0-0.1 M concentration and 20-40 °C.

5.1.2.3. The Conductivity and Concentration Relations

The conductivity of the reaction mixture changes with conversion and therefore the extent of the reaction can be monitored by recording the conductivity with respect to time. A calibration curve is needed to relate conductivity data to concentration values.

5.1.3. Experimental Setup

The apparatus used in this experiment is shown in Figures 5.1.1 and 5.1.2. The plug flow reactor is 0.4 L.

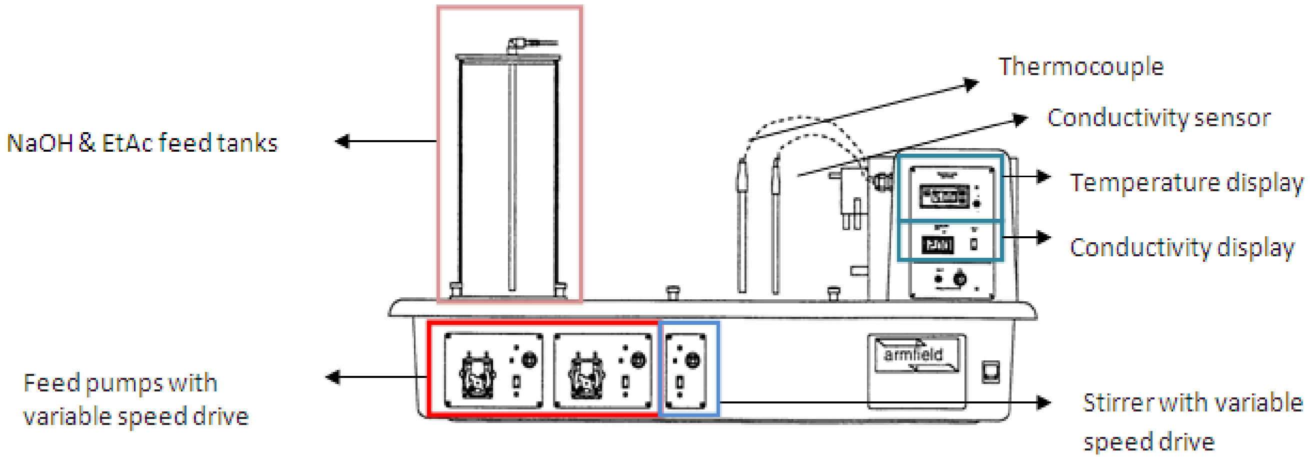

Figure 5.1.1. Chemical reactor service unit.

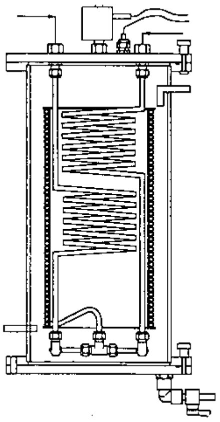

Figure 5.1.2. Tubular reactor.

5.1.4. Procedure

1. Prepare 100 ml of 0.05 M NaOH solution in a 1000 ml beaker, record conductivity data.
2. Add 100 ml distilled water to the beaker to dilute the NaOH solution, make sure it is perfectly mixed, and record conductivity data. Repeat this step six more times to prepare a calibration curve.
3. Prepare 5 L of 0.05 M ethyl acetate and 0.05 M NaOH solutions. Pour these solutions into the feed tanks.
4. Adjust a constant flow rate by setting the pump speeds of both reactants.
5. Record the conductivity when steady state is reached.
6. Repeat the same procedure for a different flow rate and for the same flow rate again.

Safety Issues: In this experiment, sodium hydroxide (NaOH) and ethyl acetate (EtAc) will be used as reactants. NaOH is poisonous and corrosive. It may be fatal if swallowed and harmful if inhaled. It causes burns to any area of contact and reacts with water, acids and other materials. EtAC is a flammable liquid and vapor. It causes eye irritation. Breathing it may cause drowsiness and dizziness. It may also cause respiratory tract irritation. Prolonged or repeated contact causes defatting of the skin with irritation, dryness, and cracking. During the experiment, beware of risks when handling with reactants. Make sure all the tanks are emptied, and all the electronic devices are unplugged at the end of the experiment. In case of eye or skin contact, remove any contact lenses or contaminated clothing or shoes. Immediately flush eyes or skin with plenty of cold water for at least 15 minutes. Cover the irritated skin with an emollient. In case of inhalation, remove to fresh air. If breathing is difficult get medical attention immediately. In case of ingestion, do not induce vomiting. Never give anything by mouth to an unconscious person. For further information, check MSDS of sodium hydroxide and ethyl acetate [4, 5]. The solutions used in this experiment are dilute in terms of the chemicals, therefore no need to a special treatment.

5.1.5. Report Objectives

1. Solve Eq. 5.1.8 for rate constant, k. Show your work in detail.
2. Calculate rate constant.
3. Make error analysis, i.e. compare two results of repeated experiments, and compare the rate constant found with theoretical k value at room temperature and atmospheric pressure

References

1. Perry, R.H. and D. Green, *Perry's Chemical Engineers' Handbook*, 8th edition, Mc Graw-Hill, New York, 2008.
2. Levenspiel, O., *Chemical Reaction Engineering,* 3rd edition, Cambridge University, 1999.
3. Fogler, H. S., *Elements of Chemical Reaction Engineering,* 4th edition, Prentice-Hall Inc., 2006.
4. Sodium Hydroxide MSDS, http://www.sciencelab.com/msds.php?msdsId=9924998.
5. Ethyl Acetate MSDS, http://www.sciencelab.com/msds.php?msdsId=9927165.

5.2. DETERMINATION OF KINETIC PARAMETERS OF THE SAPONIFICATION REACTION IN A CSTR

Keywords: *Continuous stirred tank reactors, saponification, mathematical modeling, differential equations.*

Before the experiment: *See your TA. Read the booklet carefully. Be aware of the safety precautions. Make sure to do all solution preparation calculations before you come to lab.*

Ethyl Acetate Mol wt.: 88.10, Density: 0.898 g/cm^3 (liquid)
Sodium Hydroxide Mol wt.: 40.00 (pellet)

5.2.1. Aim

To study the dynamics of a CSTR during different stages of its continuous operation by using the saponification of ethyl acetate reaction.

5.2.2. Theory

5.2.2.1. Continuous-Stirred Tank Reactors

Continuous-stirred tank reactors (Fig. 5.2.1) are used very commonly in industrial processes. For this type of reactor, mixing is complete, so that the temperature and the composition of the reaction mixture are uniform in all parts of the vessel and are the same as those in the exit stream [1].

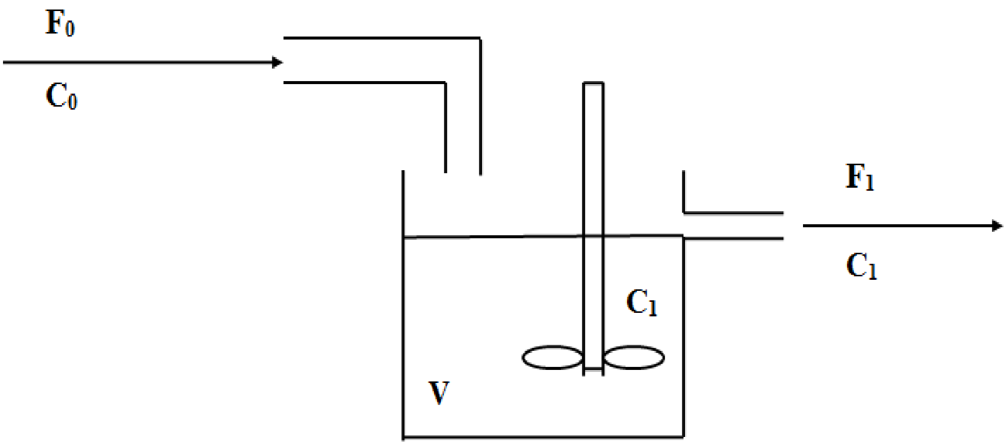

Figure 5.2.1. Continuous stirred tank reactor.

Three stages of the continuous operation of a CSTR can be modeled.

1. From beginning to overflow
2. From overflow to steady state
3. Steady state operation

The first and second stages are transient and they produce differential equations. The third stage is represented by a steady state model which contains algebraic equations.

Stage One

This stage is semibatch. There is no output because the reactor contents do not yet reach the overflow level. With assuming that the saponification reaction of ethyl acetate with sodium hydroxide is second order overall, a material balance on either NaOH or ethyl acetate (both reactants are at the same concentration and flow rate) gives Eq. 5.2.1 or 5.2.2:

rate of accumulation = rate of input - rate of consumption

$$\frac{d(VC)}{dt} = vC_0 - VkC^2 \tag{5.2.1}$$

or

$$V\frac{dC}{dt} + C\frac{dV}{dt} = vC_0 - VkC^2 \tag{5.2.2}$$

where

C = concentration	(M)
C_0 = initial concentration	(M)
v = volumetric flow rate	(L/min)
k = reaction rate constant	
t = time	(min)
V = volume of reactor	(L)

But ‘V’ is a function of time, and since the system is of constant density and flow rate, a total mass balance gives:

$$\frac{dV}{dt} = v \qquad \text{or} \qquad V = vt$$

since at $t = 0$, $V = 0$. Eq. 5.2.2 gives Eq. 5.2.3

$$\frac{dC}{dt} = \frac{C_0}{t} - \frac{C}{t} - kC^2 \qquad (5.2.3)$$

Eq. 5.2.3 is subject to $C = C_0$ at $t = 0$.

Stage Two

The second stage is continuous but not yet steady. The concentration is changing with time but the volume of the reactants is constant. A material balance takes the form of equations 5.2.4 and 5.2.5

rate of accumulation = rate of input - rate of output - rate of consumption

$$V\frac{dC}{dt} = vC_0 - vC - VkC^2 \qquad (5.2.4)$$

and therefore,

$$\frac{dC}{dt} = \frac{C_0}{t} - \frac{C}{t} - kC^2 \qquad (5.2.5)$$

where

$T = t - \tau$ (min)

$t = V/v$ (min)

At steady state, $C = C_s$, which is a particular solution to Eq. 5.2.5.

Stage Three

This is the easiest stage to model. A material balance results in equations 5.2.6 and 5.2.7

rate of input = rate of output + rate of consumption

$$vC_0 = vC_s + VkC_s{}^2 \qquad (5.2.6)$$

$$k\tau C_s{}^2 + C_s - C_0 = 0 \qquad (5.2.7)$$

The calculation of the specific rate constant k can be carried out by the Eq. 5.2.8,

$$k = \frac{(v_{A}+v_{B})}{V}\frac{(C_{A0}-C_{A})}{C_{A}^{2}} \qquad \text{L / mol.s} \qquad (5.2.8)$$

For a reactant A in a reactor operating at steady state, the volume (V) may be assumed constant and the steady state concentration of NaOH in the reactor (C_A) may be used to calculate the specific rate constant (k) [2, 3].

In this experiment, the kinetic parameters of the saponification reaction will be calculated based on the conductivity data collected during the experiment performed in a CSTR, and the results will be compared with the literature. Using a computational tool, NaOH concentration on stream and the rate constant will be determined and compared with the experimental data.

5.2.2.2. The Conductivity and Concentration Relations

The conductivity of the reaction mixture changes with conversion and therefore the extent of the reaction can be monitored by recording the conductivity with respect to time. A calibration curve is needed to relate conductivity data to concentration values.

5.2.3. Experimental Setup

The apparatus used in this experiment is shown in Figures 5.2.2 and 5.2.3. The reactor volume in this experiment is 1.6 L.

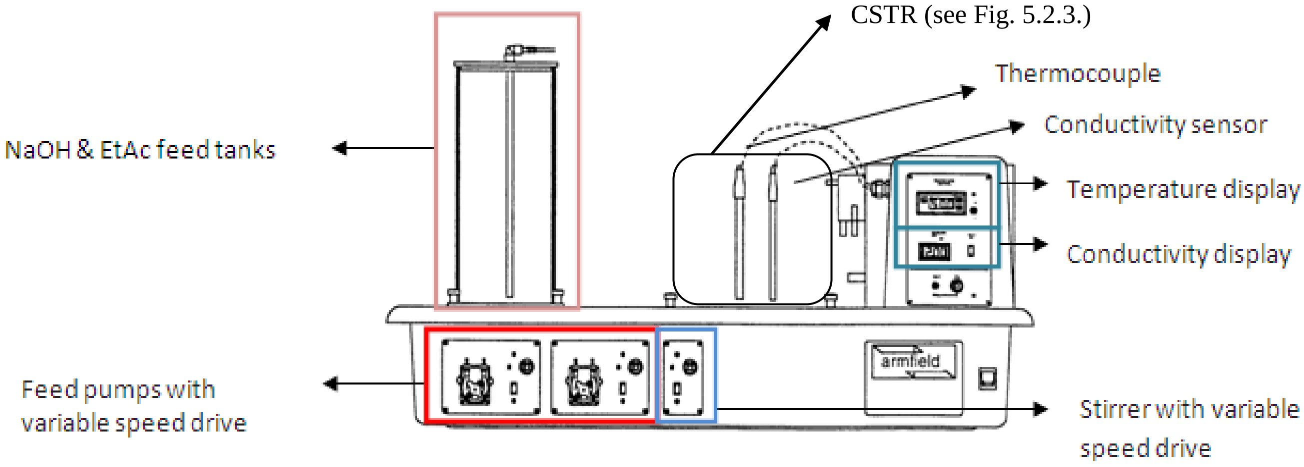

Figure 5.2.2. Chemical reactor service unit.

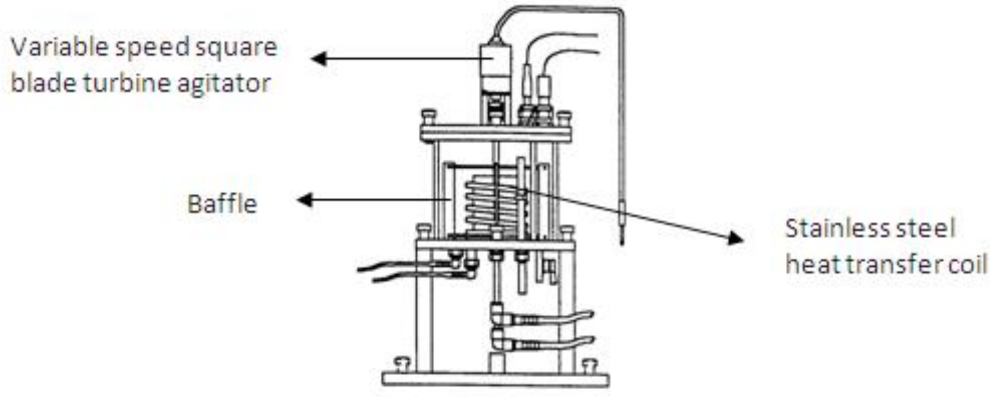

Figure 5.2.3. Continuous stirred tank reactor.

5.2.4. Procedure

1. Prepare 100 ml of 0.05 M NaOH solution in a 1000 ml beaker, record conductivity data.
2. Add 100 ml distilled water to the beaker to dilute the NaOH solution, make sure it is perfectly mixed, and record conductivity data. Repeat this step six more times to prepare a calibration curve.
3. Make up 5 liter batches of 0.05 M sodium hydroxide and 0.05 M ethyl acetate.
4. Remove the lids of the reagent vessels and carefully fill the reagents. Refit the lids.
5. Set the pump speeds of both reactants to give 50 ml/min flow rate.
6. Set the agitator speed controller to 7.0.
7. Switch on the feed pumps and agitator motor. Start the stopwatch.
8. Collect conductivity data each minute for 45 minutes.

Safety Issues: In this experiment, sodium hydroxide (NaOH) and ethyl acetate (EtAc) will be used as reactants. NaOH is poisonous and corrosive. It may be fatal if swallowed and harmful if inhaled. It causes burns to any area of contact and reacts with water, acids and other materials. EtAC is a flammable liquid and vapor. It causes eye irritation. Breathing it may cause drowsiness and dizziness. It may also cause respiratory tract irritation. Prolonged or repeated contact causes defatting of the skin with irritation, dryness, and cracking. During the experiment, beware of risks when handling with reactants. Make sure all the tanks are emptied, and all the electronic devices are unplugged at the end of the experiment. In case of eye or skin contact, remove any contact lenses or contaminated clothing or shoes. Immediately flush eyes or skin with plenty of cold water for at least 15 minutes. Cover the irritated skin with an emollient. In case of inhalation, remove to fresh air. If breathing is difficult get medical attention immediately. In case of ingestion, do not induce vomiting. Never give anything by mouth to an unconscious person. For further information, check

MSDS of sodium hydroxide and ethyl acetate [4, 5]. The solutions used in this experiment are dilute in terms of the chemicals, therefore no need to a special treatment.

5.2.5. Report Objectives

You may assume that the saponification reaction of ethyl acetate with sodium hydroxide is second order overall.

1. Prepare a calibration chart for NaOH concentration and conductivity.
2. Prepare a spreadsheet to calculate sodium hydroxide concentration, sodium acetate concentration and the degree of conversion of sodium hydroxide and sodium acetate for each of the conductivity data taken over the period of the experiment.
3. Draw sodium hydroxide concentration versus time, sodium acetate concentration versus time, and the degree of conversion of sodium hydroxide versus time graphs.
4. Calculate experimental specific rate constant (k) from material balance and compare it with the one obtained from Arrhenius equation using the data found from literature.
5. Draw sodium hydroxide concentration versus time using MATLAB starting from differential equation obtained from material balance, estimate steady state concentration of sodium hydroxide and compare it with the experimental one.
6. Derive all of the equations you use in the theory part.

References

1. Fogler, H. S., *Elements of Chemical Reaction Engineering*, 4th edition, Prentice-Hall Inc., 2006.
2. Levenspiel, O., *Chemical Reaction Engineering,* 3rd edition, Cambridge University, 1999.
3. Perry, R.H., and D. Green, *Perry's Chemical Engineers' Handbook*, 7th edition, Mc Graw-Hill, New York, 1997.
4. Sodium Hydroxide MSDS, http://www.sciencelab.com/msds.php?msdsId=9924998.

Ethyl Acetate MSDS, http://www.sciencelab.com/msds.php?msdsId=9927165.

5.3. EXPERIMENTAL AND NUMERICAL DETERMINATION OF KINETIC PARAMETERS OF A REACTION IN A SERIES OF CSTRS

Keywords: *CSTR, CSTR in series, saponification, conversion.*

Before the experiment: *Make sure to do all solution preparation calculations before you come to lab. For further information about the chemicals, look over [1, 2].*

Ethyl Acetate Mol wt.: 88.10, Density: 0.898 g/cm^3 (liquid)
Sodium Hydroxide Mol wt.: 40.00 (pellet)

5.3.1. Aim

To observe transient changes in concentrations of three CSTRs in series using of experimental measurements and computational methods and to determine the rate constant of the saponification reaction under steady state conditions.

5.3.2. Theory

In continuously operated chemical reactors, the reactants are pumped at constant rate into the reaction vessel and the chemical reaction takes place as the reaction mixture flows. The reaction products are continuously discharged to the subsequent separation and purification stages. The extent of the required separation and purification process depends on the efficiency of the reactor, and so the selection of the correct type of the reactor for a given duty is most important since the economics of the whole process could hinge on this choice. Normally, the efficiency of a chemical reactor is measured by its ability to convert the reactants into the desired products with the exclusion of unwanted by-products; this is measured by yield. However, additional factors such as safety, ease of control and stability of the process must also be considered. Many of these factors depend on the size and shape of the reactor. The size of reactor for a purposed feed rate depends on the reaction kinetics of the materials undergoing chemical change and on the flow conditions in the reactor. On the other hand, the flow conditions are determined by the cross sectional area of the path through which the reaction mixture flows; i.e. the shape of the reactor. Thus, it is apparent that size and shape are interrelated factors, which must be taken together when considering continuous reactors [3].

5.3.2.1. Continuously Stirred Tank Reactors (CSTRs)

CSTRs are usually cylindrical tanks with stirring provided by agitators mounted on a shaft inserted through the vessel lid. In addition, the tank is fitted with auxiliary equipment necessary to maintain the desired reaction temperature and pressure conditions [3].

The well-stirred tank reactor is used mostly for liquid phase reactions. In normal operation, a steady continuous feed of reactants is pumped into the vessel and since there is usually negligible density change on reaction, an equal volume of the reactor contents is displaced through an overflow pipe situated near the top of the vessel [3].

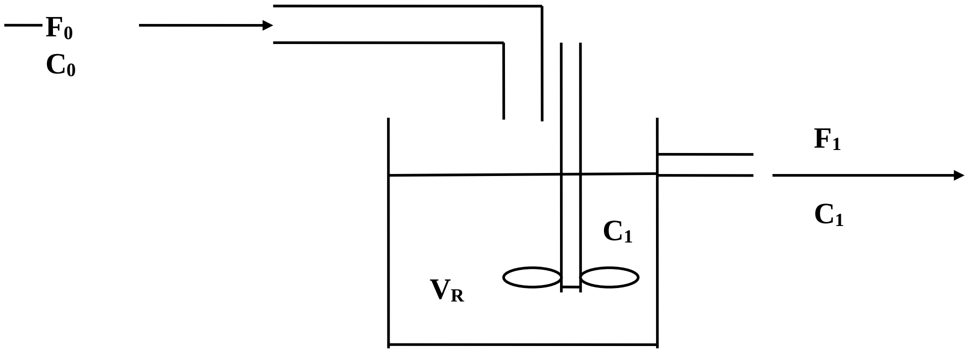

Figure 5.3.1. Single continuous stirred tank reactor.

For a single stirred tank reactor (Figure 5.3.1), it is assumed that the design of the agitator provides complete mixing of the vessel contents to achieve uniform temperature and composition distribution throughout the vessel. This premise of complete mixing then implies that the reactor outlet stream is identical in temperature and composition to the bulk reactor contents [4].

For an effective reactor volume ‘V’, molar input and output ‘F’, and moles N the mole balance for component A is given by Eq. 5.3.1:

$$F_{A0} - F_{A1} + r_A V_R = \frac{dN_A}{dt} \tag{5.3.1}$$

For an irreversible reaction, the reaction rate term defined as Eq. 5.3.2 [3]:

$$r_A = k{C_{A1}}^n \tag{5.3.2}$$

The reaction rate r_A is constant within the reactor and time when steady state operation has been established. The right hand side of the Equation 5.3.1 vanishes under steady state operation therefore the equation becomes algebraic.

The conversion of the reactant can be defined as Eq. 5.3.3:

$$x = \frac{F_{A0} - F_{A1}}{F_{A0}} \tag{5.3.3}$$

Combining equations 5.3.1 and 5.3.3 under steady-state conditions, the design equation of a single CSTR is obtained as Eq. 5.3.4 [4].

$$V_R = F_{A0}\,\frac{x}{-r_A} \tag{5.3.4}$$

Single Tanks with Simple Reactions

For a first order reaction under steady state conditions, dividing Eq. 5.3.1 by volumetric flow rate yields $Q\ (volume/time)$ as in Eq. 5.3.5 [3]:

$$C_{A0} = C_{A1}\left(1 + \frac{kV_R}{Q}\right) \tag{5.3.5}$$

V_R/Q is the space time and will be given the symbol 'τ'. Hence, Eq. 5.3.6 forms as

$$\frac{C_{A1}}{C_{A0}} = \frac{1}{(1 + k\tau)} \tag{5.3.6}$$

Since the input and the outlet volumetric flow rates are equal, the conversion 'x' can also be written as Eq. 5.3.7:

$$x = \frac{C_{A0} - C_{A1}}{C_{A0}} = 1 - \frac{1}{(1 + k\tau)} \tag{5.3.7}$$

and as is usual with first order reactions the result is independent of the feed concentration.

For a second order reaction starting from the overall mole balance around each tank individually at steady state conditions, Equation 10.3.1 under equimolar feed becomes as Eq. 5.3.8:

$$C_{A0} = C_{A1} + k\tau {C_{A1}}^{2} \tag{5.3.8}$$

and the positive root of this quadratic equation gives Eq. 5.3.9:

$$C_{A1} = \frac{\left(-1 + \sqrt{1 + 4k\tau C_{A0}}\right)}{2k\tau} \tag{5.3.9}$$

hence the conversion equation becomes as Eq. 5.3.10,

$$x = 1 + \frac{-1 + \sqrt{1 + 4k\tau C_{A0}}}{2k\tau C_{A0}} \tag{5.3.10}$$

Transient Behavior

Under unsteady state conditions the mass balance turns out to be an ordinary differential equation that can be solved numerically in order to simulate the theoretical behavior of concentration and conversion with respect to time. For a second order reaction this equation is derived from the Eq. 5.3.1 by substituting the expressions of concentration, space time, and conversion as Eq. 5.3.11 [4].

$$\frac{dx}{dt} = kC_{A0}(1-x)^2 - \frac{x}{\tau} \tag{5.3.11}$$

where
x = conversion of reactant A
C_{A0}= Initial concentration of A
k = Reaction rate constant
τ = Space time (V/Q)

Multiple Tank Cascade with Simple Reactions (CSTRs in Series)

A major shortcoming of a single stirred tank is that all of the reaction takes place at the low final reactant concentration and hence requires an unduly large reactor hold-up. If a number of smaller well-stirred reactors are arranged in series, only the last one will have a reaction rate governed by the final reactant concentration and all of the others will have higher rates. Hence, for a given duty the total reactor hold-up will be less than for a single tank. This saving in reactor volume increases as the required fractional conversion increases and also as the number of installed tanks increases. In fact, all of the desirable features of the CSTR may be retained while the low hold-up characteristics of a plug flow tubular reactor are approached, e.g. five to ten tanks in a cascade are likely to give high conversion values at low hold-up times similar to a pug-flow reactor. It is a matter of economics to balance the cost of the number of tanks against their reduced size [3].

There are other operational advantages in carrying out reactions in series of stirred tanks. For example if one vessel in the cascade has to be put out of commission for any reason, it may be bypassed and production continued at a slightly reduced rate whereas failure of a single CSTR would entail complete loss in production [3].

5.3.2.2. Saponification Reaction

$$NaOH \quad + \quad CH_3COOC_2H_5 \quad \rightarrow \quad CH_3COONa \quad + \quad C_2H_3OH$$

Sodium Hydroxide + *Ethyl Acetate* → *Sodium Acetate* + *Ethyl Alcohol*
(A) *(B)* *(C)* *(D)*

The reaction can be considered first order with respect to sodium hydroxide and ethyl acetate i.e. second order overall, within the limits of concentration (0-0.1M) and temperature (20-40˚C) studied [5].

To calculate the specific rate constant k, the overall mass balance may be written as [4]:

Rate of change within the reactor = Input – Output + Accumulation

i.e. for NaOH in a reactor operating at steady state the volume may be assumed constant. The steady state concentration of NaOH in reactor (C_A) may be used to calculate the specific rate constant (k) as in Eq. 5.3.12 and Eq. 5.3.13:

$$k = \frac{Q}{V}\frac{(C_{A0} - C_A)}{C_A^2} \tag{5.3.12}$$

$$k = \frac{(Q_A + Q_B)}{V}\frac{(C_{A0} - C_A)}{C_A^2} \tag{5.3.13}$$

5.3.2.3. Conductivity and Concentration Relations

The conductivity of the reaction mixture changes with conversion and therefore the extent of the reaction can be monitored by recording the conductivity with respect to time. Conductivity data obtained throughout the experiment has to be converted into concentration data of the system. A calibration chart showing the relation between the conductivity of the fluid and the concentration of the ionized material can be obtained by measuring known concentrations of the material's conductivity.

The reaction carried out in a Continuous Stirred Tank Reactor or series CSTRs eventually reaches steady state when a certain amount of conversion of the starting reagents has taken place. The steady state conditions will depend on concentration of reagents, flow rate, volume of reactor and temperature of reaction.

In this experiment, the reaction rate constant for the saponification reaction will be calculated based on the conductivity data collected during the experiment carried on three CSTR in series and compared with the literature value. In addition, the final conversion will calculated numerically using suitable computational tools.

5.3.3. Experimental Setup

The experimental setup used in this experiment is shown in Figure 5.3.2.

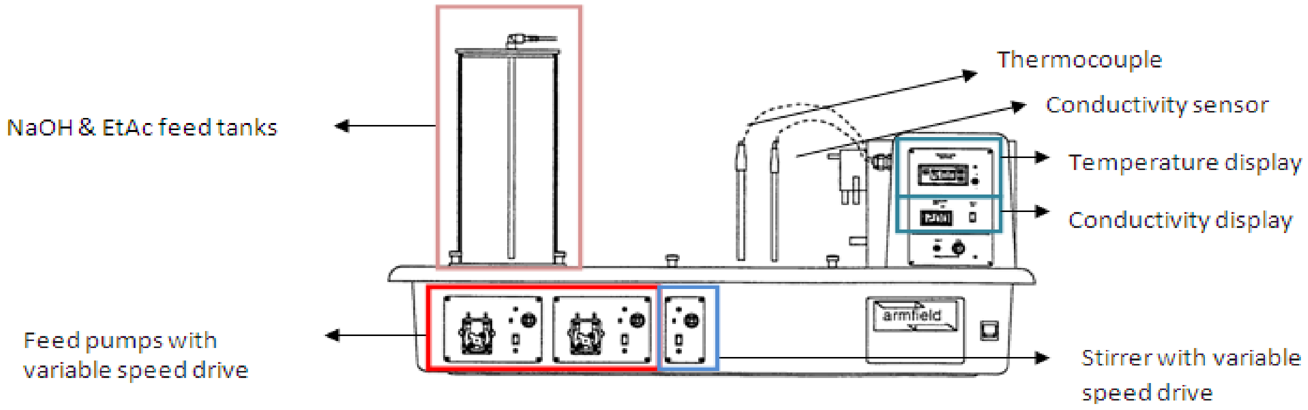

Figure 5.3.2. Chemical reactor service unit.

5.3.4. Procedure

1. Prepare a calibration curve for the conductivity vs. concentration of NaOH (for the solutions with the concentrations 0.005M, 0.01M, 0.02M, 0.03M, 0.04M, 0.05M).
2. Prepare 3.0 liter batches of 0.05M sodium hydroxide and 0.05M ethyl acetate.
3. Remove the lids of the reagent tanks and carefully, fill with the reagents. Refit the lids.
4. Set the pump speed control to give 50 ml/min flow rate.
5. Start agitators.
6. Switch on both feed pumps and agitator motor, and start recording conductivity.
7. Collect conductivity data for 30 minutes in 30 seconds intervals.

Safety Issues: In this experiment, sodium hydroxide (NaOH) will be used as reactant. NaOH is poisonous and corrosive. It may be fatal if swallowed and harmful if inhaled. It causes burns to any area of contact and reacts with water, acids and other materials Prolonged or repeated contact causes defatting of the skin with irritation, dryness, and cracking. During the experiment, beware of risks when handling with reactant. Make sure all the tanks are emptied, and all the electronic devices are unplugged at the end of the experiment. In case of eye or skin contact, remove any contact lenses or contaminated clothing or shoes. Immediately flush eyes or skin with plenty of cold water for at least 15 minutes. Cover the irritated skin with an emollient. In case of inhalation, remove to fresh air. If breathing is difficult get medical attention immediately. In case of ingestion, do not induce vomiting. Never give anything by mouth to an unconscious person. For further information, check MSDS of sodium hydroxide and ethyl acetate [6]. The solutions used in this experiment are dilute in terms of the chemicals, therefore no need to a special treatment. After the experiment make sure all the tanks are emptied, and all the electronic devices are unplugged.

5.3.5. Report Objectives

1. Find the reaction rate constants for each CSTR starting from the design equation of a CSTR.
2. Find the rate constant of the reaction from the literature and calculate the error.
3. Find the NaOH conversion corresponding to each measurement.
4. Draw conversion vs time graphs for each reactor during the whole experiment (Draw on the same graph).
5. Solve the differential equations numerically to find the conversions using MATLAB or POLYMATH software (Use literature value for the reaction rate constant).
6. Compare the conversion values obtained from numerical solution with experimental observations, showing experimental and numerical conversions on a single graph.

References

1. http://akkimyaas.com/urunler/aspx.
2. http://www.merckmillipore.com/pharmaceutical-ingredients/
3. Cooper, A. R. and G. V. Jeffreys, *Chemical Kinetics and Reactor Design*, Oliver & Boyd, Norwich, 1971.
4. Fogler, H. G., *The Elements of Chemical Reaction Engineering*, 2nd edition, Prentice Hall, New York, 1992.
5. Perry, R. H. and D. Green, *Perry's Chemical Engineers' Handbook*, 6th edition, Mc Graw-Hill, New York, 1988.
6. Sodium Hydroxide MSDS, http://www.sciencelab.com/msds.php?msdsId=9924998.