

KINETICS OF SODIUM HYDROXIDE AND ETHYL ACETATE REACTION IN A CONTINUOUS STIRRED TANK REACTOR: A COMPARISON OF EXPERIMENTAL AND THEORETICAL CONVERSION

S M Nazmuz Sakib^{1, 2, 3*}

¹Graduate of BSc in Business Studies, School of Business and Trade Pilatusstrasse 6003, 6003 Luzern,

²Graduate of LLB (Hon's), Faculty of Law Dhaka International University,

³Graduate of MBA (Human Resources), International MBA Institute,

Article Info

*Corresponding Author

Email Id:sakibpedia@gmail.com

Keywords

Kinetics, sodium hydroxide, space, conversion, theoretical

Abstract

In this experiment, the kinetics of the reaction between sodium hydroxide and the ethyl acetate is studied. Both the reactants are fed to the continuous stirred reactor and the conductivities are measured. These conductivities are then used to find out the conversion, reaction time or the reaction rate constant as well the as the reaction rate using the equations from literature. Graph is plotted between the space time and conversion and the relationship between the space time and conversion is analyzed and compared with the theoretical one.



1.Introduction

The continuous stirred tank reactor is used for the reaction which involves chemical reaction in chemical process plants. It uses the agitator which is in continuous operation to make it a mixed-flow reactor or continuous stirred reactor. The reaction which is to be studied in this regard is first order sodium hydroxide and ethyl acetate reaction. Sodium hydroxide and ethyl acetate reacts to form sodium acetate and ethyl alcohol as follows: $\text{NaOH} + \text{H}_3\text{COOC}_2\text{H}_5 \rightarrow \text{CH}_3\text{COONa} + \text{C}_2\text{H}_5\text{OH}$ When applying the mass balance on CSTR Input – Output

= Production $\text{FA}_{\text{in}} - \text{FA}_{\text{out}} = -r_a V$ Where the kinetic rate expression for first order reaction is $-r_a = k C_A C_B$ Where k is the reaction rate constant which depends on the temperature rather than the concentration of the reactants. The conversion of the reactant A is calculated by the following expression: $X_a = \frac{\text{Ca}(\text{in}) - \text{Ca}(\text{out})}{\text{Ca}(\text{in})}$ This conversion is helpful to find out the overall rate of reaction and to examine the relationship between the t and x for CSTR. The flow rate of the CSTR can be calculated by using the following equation: $\text{Fa} = \text{Ca} v$ The volume used in the above equation is

given by: $v_{in} - v_{out} = v$ The ratio of reactor volume and the inlet volumetric flowrate is called the space time and is given by the following equation: $t=V/v$ The above equation shows the reaction time in the reactor. The following expression is obtained by the substitution of above equations in the overall mass balance equation.

$$\tau k = Ca(in) - Ca(out) / Ca(out)^2$$

$$\tau k = Xa / C(in)(1 - Xa)^2$$

The rate of reaction can be calculated by the following expression:

$$-ra = k * Ca^2$$

the relationship between the conductivity and the temperature is given by the following expression which is for the sodium acetate, the product of under-studied reaction. $A_{SA} = 0.070[1 + 0.0284(T - 294)] C_{SA}$ for $T > 294$ K The conductivity of the sodium hydroxide solution is given by the following expression: $A_{SH} = 0.195[1 + 0.0184(T - 294)] C_{SH}$ for $T > 294$ K the measured conductivity is the sum of above two conductivities

$$aSA = A_{SA} + A_{SH}$$

this can be related to the concentration and conversion using the stoichiometric table.

1.1 Experimental part

1. Before starting the experiment, have a conversation with the technician.
2. The solutions are already in the tank so after they run out asks your technician to refill it.
3. Turn of the hot water circulator and adjust the temperature of PID controller to 30 degrees Celsius.
4. Turn the automatic mode of operation of PID.
5. The flowrate is set to be 40ml/min of the pump.
6. The concentrations of both solutions and the volumes of the reactor are filled in the respective boxes in the software.
7. Turn on the power button and wait for 35 to 45 mins till the steady state is achieved.
8. Once the steady state is achieved start taking the readings of the conductivity.
9. Save the data on excel file and repeat the above steps by changing the temperatures to 35 and 40 degrees Celsius.

1.2 Results and discussion

1.2.1 Calculations

Table 1: Observation table for the experiment.

Run	C _o (M)	V(L)	f(ml/min)	T(K)	A(S)
1	0.05	1	40	303.6	0.00769
2	0.05	1	50	303.3	0.00777
3	0.05	1	60	303.4	0.00792
4	0.05	1	70	303.1	0.00803
5	0.05	1	80	303.4	0.00815

The first part of calculations goes like that: First, we will suppose the outlet concentration of A and then calculate the conversion using the following equation: $Xa = Ca(in) - Ca(out) / Ca(in)$ Then the

outlet concentration of B is also calculated using the equation: $Cb(out) = Cb(in) - Ca(in) * X$ The conductivities are measured using the above parameters and the following equations: $A_{SA} =$

0.070[1+0.0284(T-294)] C_{SA} for T>294 K A_{SH} = conductivity. If the error is less than the Ca(out) is
 0.195[1+0.0184(T-294)] C_{SH} for T> 294 K Both correct otherwise do iteration till the error get
 the above conductivities are added and compared negligible. The graph is plotted for different
 with the experimental value of thermal values of temperature.

The detailed calculations are: Suppose Ca(out) is 0.0128 X_a = Ca(in) – Ca(out)/Ca(in)= 0.05-0.0128/0.05 = 0.744
 C_b(out)= C_b(in) – Ca(in)*x = 0.05- (0.05*0.744) = 0.0128 A_{SA} = 0.070[1+0.0284(T-294)] C_{SA} = 0.070[1+0.0284(303.6-
 294)] *0.0128 = 0.002937
 A_{SH} = 0.195[1+0.0184(T-294)] C_{SH} = 0.070[1+0.0284(303.6-294)] * 0.0128 = 0.001140285 At = 0.002937+
 0.001140285= 0.004077 A-At = 0.00769-0.004077 = 0.003612821 Suppose Ca(out) is 0.0129 X_a = Ca(in) –
 Ca(out)/Ca(in)= 0.05-0.0129/0.05 = 0.744 C_b(out)= C_b(in) – Ca(in)*x = 0.05- (0.05*0.744) = 0.0129 A_{SA} =
 0.070[1+0.0284(T-294)] C_{SA} = 0.070[1+0.0284(303.3-294)] *0.0129 = 0.002946
 A_{SH} = 0.195[1+0.0184(T-294)] C_{SH} =
 0.070[1+0.0284(303.3-294)] * 0.0129 = 0.0011415
 At = 0.002946+ 0.0011415 = 0.004087 A-At = 0.00777- 0.004087= 0.003682547 Suppose Ca(out) is 0.013 X_a = Ca(in) –
 Ca(out)/Ca(in)= 0.05-0.013/0.05 = 0.74 C_b(out)= C_b(in) – Ca(in)*x = 0.05- (0.05*0.74) = 0.013 A_{SA} =
 0.070[1+0.0284(T-294)] C_{SA} = 0.070[1+0.0284(303.4-294)] *0.013 = 0.002973 A_{SH} = 0.195[1+0.0184(T-294)] C_{SH} =
 0.070[1+0.0284(303.4-294)] * 0.013 = 0.001152934 At = 0.002973+ 0.001152934 = 0.004126 A-At = 0.00792 -
 0.004126=0.003793613 Suppose Ca(out) is 0.0131X_a = Ca(in) – Ca(out)/Ca(in)= 0.05-0.0131/0.05 = 0.738 C_b(out)=
 C_b(in) – Ca(in)*x = 0.05- (0.05*0.738) = 0.0131 A_{SA} = 0.070[1+0.0284(T-294)] C_{SA} = 0.070[1+0.0284(303.1-294)]
 *0.0131 = 0.002982
 A_{SH} = 0.195[1+0.0184(T-294)] C_{SH} = 0.070[1+0.0284(303.1-294)] * 0.0131 = 0.001153989 At = 0.002982+ 0.001153989
 = 0.004136 A-At = 0.00803 - 0.004136=0.003893785 Suppose Ca(out) is 0.0132
 X_a = Ca(in) – Ca(out)/Ca(in)= 0.05-0.0132/0.05 = 0.736 C_b(out)= C_b(in) – Ca(in)*x = 0.05- (0.05*0.736) = 0.0132 A_{SA} =
 0.070[1+0.0284(T-294)] C_{SA} = 0.070[1+0.0284(303.4-294)] *0.0132 = 0.003019 A_{SH} = 0.195[1+0.0184(T-294)] C_{SH} =
 0.070[1+0.0284(303.4-294)] * 0.0132 = 0.001170671 At = 0.003019+ 0.001170671 = 0.00419 A-At = 0.00815 - 0.00419
 = 0.00396013

Table 2

Run	Ca(in)(M)	Cb(in)(M)	V(L)	f(ml/min)	T(K)	A(S)
1	0.05	0.05	1	40	303.6	0.00769
2	0.05	0.05	1	50	303.3	0.00777
3	0.05	0.05	1	60	303.4	0.00792
4	0.05	0.05	1	70	303.1	0.00803
5	0.05	0.05	1	80	303.4	0.00815

Calculations for the outlet concentration of A						
Ca(out) (M)	Cb(out) (M)	x	Aa (S)	Ab(S)	At(S)	At-A
0.0128	0.0128	0.744	0.002937	0.001140285	0.004077	0.003612821
0.0129	0.0129	0.742	0.002946	0.0011415	0.004087	0.003682547

0.013	0.013	0.74	0.002973	0.001152934	0.004126	0.003793613
0.0131	0.0131	0.738	0.002982	0.001153989	0.004136	0.003893785
0.0132	0.0132	0.736	0.003019	0.001170671	0.00419	0.00396013

The difference in the calculations is Negligible. The graph is plotted as

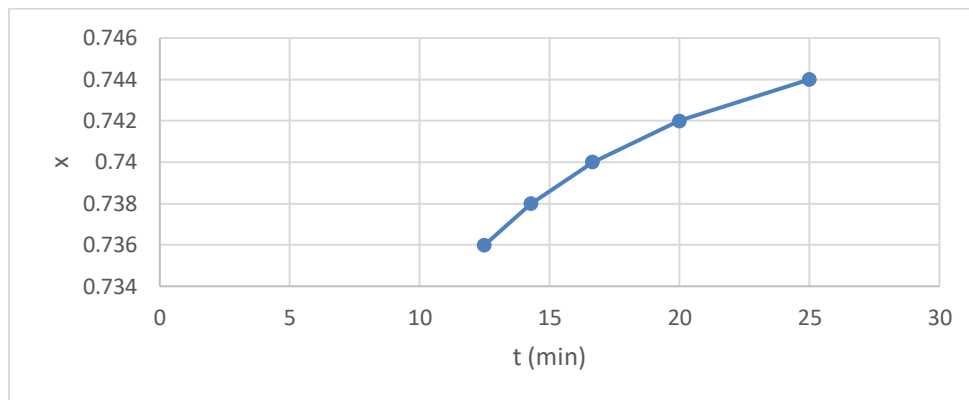


Figure 1: Graph between conversion and space time.

The second part of calculations goes like that: and plot it against the space time. The slope of the graph will give the reaction rate constant
 After calculating the Ca(out), calculate its inverse

Table 3: Calculations for k

Ca(out) (M)	1/ca(out)	t
0.0128	1/0.0128= 78.125	25
0.0129	1/0.0129= 77.51937984	20
0.013	1/0.013= 76.92307692	16.667
0.0131	1/0.0131= 76.33587786	14.2857
0.0132	1/0.0132= 75.75757576	12.5

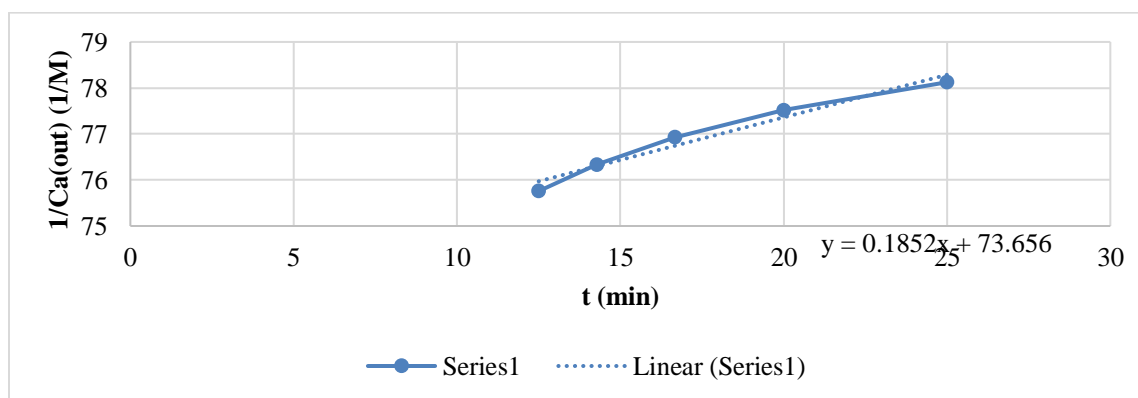


Figure 2: Graph between 1/Ca(out) and space time.

The slope of the graph gives the rate constant for the experiment and hence, the value of k is found

outtobe0.18521/M.min

Graph of Xa vs. t at specified temperatures:

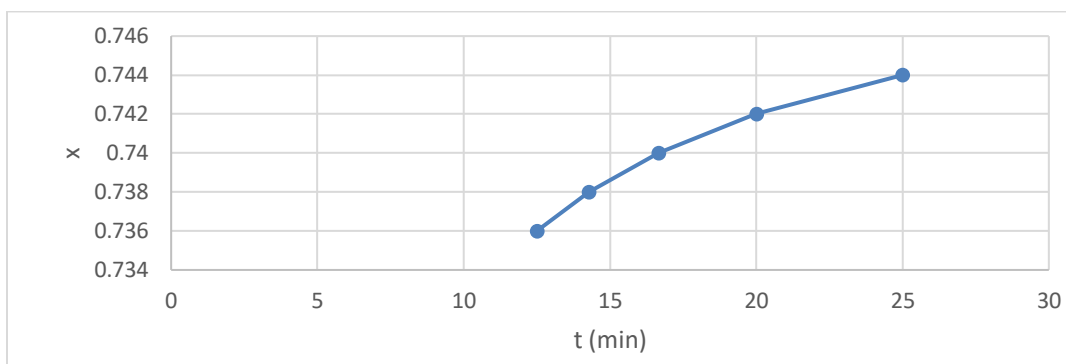


Figure 3: Graph between conversion and space time at 5 temperatures.

1.2.2 Comparison

For the comparison part, First the conversion is assumed. Then the estimated space time is calculated using the equation: $\tau = X_a / k \cdot C_{in} \cdot (1 - X_a)^2$ After that the difference between the theoretical and experimental space time is calculated. If it is negligible then the comparison between the experimental and theoretical conversion is made on the graph. The detailed calculations are as follows: Suppose that x is 0.004582 Now from the equation $\tau = X_a /$

$$k \cdot C_{in} \cdot (1 - X_a)^2 = 24.996 \quad t - t(cal) = 0.003892893$$

Suppose that x is 0.0036725 Now from the equation $\tau = X_a / k \cdot C_{in} \cdot (1 - X_a)^2 = 19.9979667 \quad t -$

$$t(cal) = 0.002033301 \quad \text{Suppose that x is } 0.003064$$

Now from the equation $\tau = X_a / k \cdot C_{in} \cdot (1 - X_a)^2 =$

$$16.6641235 \quad t - t(cal) = 0.002876534 \quad \text{Suppose that x}$$

is 0.0026283 Now from the equation $\tau = X_a /$

$$k \cdot C_{in} \cdot (1 - X_a)^2 = 14.2820031 \quad t - t(cal) =$$

0.003696855 Suppose that x is 0.00229999 Now

from the equation $\tau = X_a / k \cdot C_{in} \cdot (1 - X_a)^2 =$

$$12.489765 \quad t - t(cal) = 0.010235023$$

Table 4: Calculations for the theoretical conversion.

t	Ca(in)(M)	x(assume)	k	t(cal)	t-t(cal)
25	0.05	0.004582	0.0037	24.9961071	0.003892893
20	0.05	0.0036725	0.0037	19.9979667	0.002033301
16.667	0.05	0.003064	0.0037	16.6641235	0.002876534
14.2857	0.05	0.0026283	0.0037	14.2820031	0.003696855
12.5	0.05	0.00229999	0.0037	12.489765	0.010235023

The differences in the calculations are negligible. The graph is plotted to analyze both the Experimental and theoretical values of conversion.

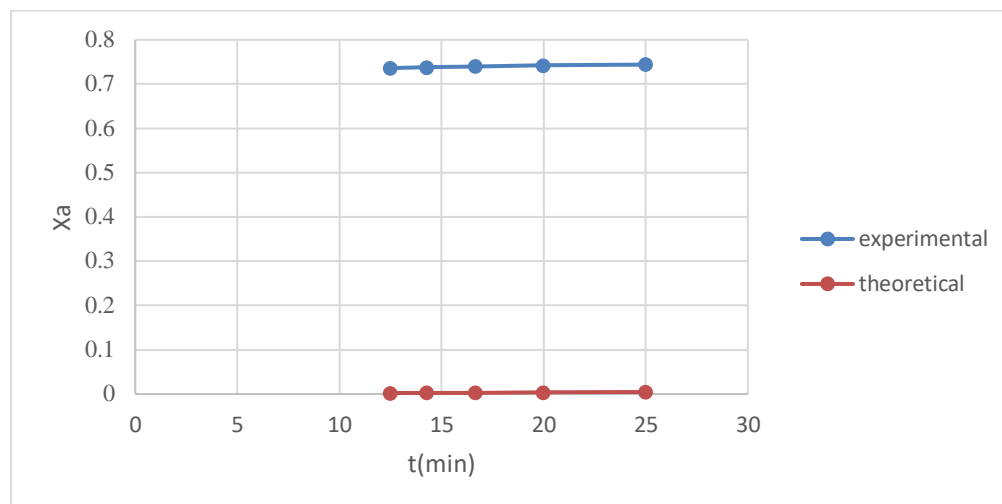


Figure 4: Comparison between experimental and theoretical conversion.

The above graph shows that at the given space time the theoretical values of conversion are far less than the experimental values of conversion. This difference in experimental and theoretical values may be due to many limitations. However, the trend of change in conversion with the change in the space time is quite similar except at the end there is a little variation in the experimental curve for conversion.

1.2.3 Limitations

The limitation to the CSTR is that it runs at small concentration and hence the small conversion occurs. When the conversion is small the reaction time or the space time is also less. It is usually operated at small industrial levels.

2. Conclusion

Sodium hydroxide is reacted with ethyl acetate in the continuous stirred tank reactor. The reaction is first order and the mass balance was performed on the reactor. After the experiment is done the conductivity is measured which then helps to find out the rate of reaction, conversion, space time and the reaction rate constant using different equations from 1 to 10. The graph between the conversion

and space time is plotted which gives us the point where the experimental graph deviates from the theoretical ones. The sources of error are human negligence, reactor not working at proper conditions or might be the environment effect like temperature is too hot or too cold.

References

- Fogler, S., 1999, *Elements of Chemical Reaction Engineering*, 3rd edition, Prentice Hall.
- Fogler, S., 1999, *Elements of Chemical Reaction Engineering*, 3rd edition, Prentice Hall.
- Levenspiel, O., 1999, *Chemical Reaction Engineering* 3rd edition, John Wiley.
- Smith, J.M., 1981, *Chemical Engineering Kinetics*, 3rd Edition, McGraw Hill.
- Streetwise, A., Heathcock, C.K., and Kosower, E.M., 1992, *Introduction to Organic Chemistry* 4th Edition, MacMillan, p 63.
- Tsijikawa, H., and Inoue, H., 1966, *Bulletin of the Chem. Soc. Of Japan*, 39, p 1837.