

MADHAV INSTITUTE OF TECHNOLOGY & SCIENCE GWALIOR (M.P)



**Department Of Chemical
Engineering**

Project Report :- Process Modelling and Simulation of Ideal Batch Reactor using MATLAB

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CERTIFICATE

This is to certify that Vaishnavi Tripathi(0901CM191057), Ritik Agrawal(0901CM191045), Chaitanya Sharma(0901CM191021), and Atharva Jain (0901CM191018), students of B. Tech. VI Semester Chemical Engineering, Madhav Institute of Technology and Science, Gwalior (M.P.) have satisfactorily completed Minor Project (170607) on "process modeling and simulation of ideal batch reactor, for the partial fulfilment of degree course in Chemical Engineering, in the academic year 2021-22.

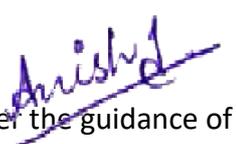
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CANDIDATE'S DECLARATION

We hereby declare that the project report – “process modelling and simulation of ideal batch reactor using matlab” which is being submitted for “Minor Project – 2 (170607) of 6th semester in “MADHAV INSTITUTE OF TECHNOLOGY & SCIENCE, GWALIOR (MP) is our genuine work done under the guidance of prof. Anish.P.Jacob, Dept. of chemical engineering, “Madhav Institute of Technology & Science”, Gwalior.

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Abstract:-

Knowledge of kinetic parameters is of extreme importance for the chemical engineer prior to design of chemical reactors. This research focuses on the study of the kinetics of the saponification reaction between sodium hydroxide and ethyl acetate in a batch reactor.

The reactions kinetics was studied through initially studying caustic soda concentrations dependency using an excess of ethyl acetate while maintaining isothermal conditions .Then the concentration dependency of ethyl acetate was evaluated using equal concentrations of reactants before operating at various condition to evaluate the temperature dependency. Analytical mathematical and computer methods were used to analyze the experimental observations and data. The results obtained (of evaluated kinetic parameters) showed, a clear agreement with the values from literature.

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Chapter 1

Introduction:-

Process Modelling

Chemical process modelling is a computer modelling technique used in chemical engineering process modelling .It typically involves using purpose-built software to define a system of interconnected components, which are then solved so that the steady state or dynamic behaviour of the system can be predicted. The system components and connections are represented as a process flow diagram .

Modelling in engineering design

Each model represents an effort to capture the process of creativity, problem solving, collaboration, and communication necessary to successfully design a solution.Each model highlights different elements of the process.

Modelling techniques

Techniques that involve collecting data from one or more sources and developing a comprehensive representation of the data in a model.

Types of models used in engineering

Mathematical models are commonly used in engineering. There are three basic classes of mathematical models: empirical, optimization, and structural. Empirical models are developed from system data.

Simulation

A simulation is a model that mimics the operation of an existing or proposed system, providing evidence for decision-making by being able to test different scenarios or process changes. This can be coupled with virtual reality technologies for a more immersive experience.

Simulations can be used to tune up performance, optimise a process, improve safety, testing theories, training staff and even for entertainment in video games! Scientifically modelling systems allows a user to gain an insight into the effects of different conditions and courses of action.

Simulation can also be used when the real system is inaccessible or too dangerous to assess or when a system is still in the design or theory stages.

Key to any simulation is the information that is used to build the simulation model and protocols for the verification and validation of models are still being researched and refined, particularly with regard to computer simulation.

How Simulation Works

Simulation works through the use of intuitive simulation software to create a visual mock-up of a process. This visual simulation should include details of timings, rules, resources and constraints, to accurately reflect the real-world process.

This can be applied to a range of scenarios, for example, you can model a supermarket and the likely behaviours of customers as they move around the shop as it becomes busier. This can inform decisions including staffing requirements, shop floor layout, and supply chain needs.

Another example would be a manufacturing environment where different parts of the line can be simulated to assess how their processes interact with those of others.

Introduction to Matlab

Matlab is a programming language similar to other well-known languages such as Java, C#, etc., which comes with its own IDE (that is Integrated Development Environment) and set of libraries. Matlab is an abbreviation of the term “Matrix Laboratory” since it was initially referred to as the matrix programming language. It is a fourth-generation programming language. It was first discovered by Cleve Moler, who at the time was the Chairman of the Computer Science department at the University of New Mexico. His goal was to find an alternative way to perform linear algebra and numerical computation for his students without them having to use Fortran. Later in 1984, Cleve Moler along with Steve Bangart and Jack Little – who recognized Matlab’s commercial potential, found MathWorks. MathWorks released its first official version of Matlab in 1984.

Uses of Matlab

1. Performing numerical linear algebra
2. Numerical computation of Matrices
3. Data analysis and visualization

4. Plotting graphs for larger data sets
5. Developing algorithms
6. Creating interfaces for the user that is the GUI- Graphical User Interface and other applications that is the API – Application Programming Interface.

Uses of Matlab

Using Matlab you can implement and design different algorithms. You can load data from different sources such as files, databases or the web to analyze your data and visualize it using Matlab visualization application which gives you a wide range of graph plots to choose from. It also makes it easier to work with larger data sets. It as a math product contains a mathematical function library that allows you to perform linear algebra and computation of matrices. This also helps to facilitate data analysis. Creating data models, prototypes, and simulations of data can be achieved. You can also design interfaces for both users as well as other programming applications to make working with Matlab easier.

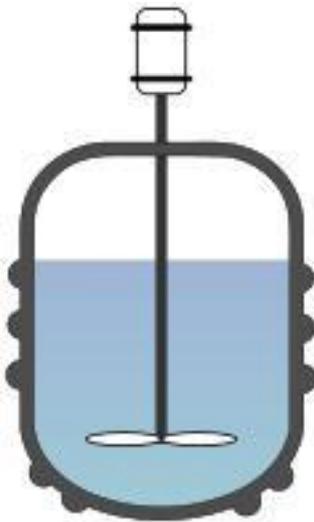
Advantages

1. It provides the fastest IDE for the mathematical computation of matrices and linear algebra.
2. Contains the best mathematical package libraries to provide support for all fields of mathematics, ranging from simple summation to matrix inversion, etc.
3. It provides multi-threading support and garbage collection to facilitate the parallel execution of algorithms.
4. Its graphics system (Simulink) includes commands for two-dimensional and three-dimensional data visualization, image processing, graphics presentation, and animation providing high-quality visualization of plots and charts.

Matlab is one of the best technologies available in the market for mathematical operations performed on matrices and linear algebra. It also provides the best support for faster and better algorithm design and testing. It makes analyzing data with different algorithms and studying the changes in behavior easy. It also provides flexibility to design new interfaces as per ones need.

Batch reactor

A batch reactor is used for small-scale operation, for testing new processes that have not been fully developed, for the manufacture of expensive products, and for processes that are difficult to convert to continuous operations. The reactor can be charged (i.e., filled) through the holes at the top.



Advantages:-

- High conversions can be obtained.
- Versatile, used to make many products.
- Good for producing small amounts.
- Easy to Clean.

Disadvantages:-

- High cost of labour per unit of production.
- Difficult to maintain large scale production.
- Long idle time (Charging & Discharging times) leads to periods of no production.

- No instrumentation – Poor product quality

Chapter2
LITERATURE SURVEY

Batch reactor design equation:-

In most batch reactors, the longer a reactant stays in the reactor, the more the reactant is converted to product until either equilibrium is reached or the reactant is exhausted. Consequently, in batch systems the conversion X is a function of the time the reactants spend in the reactor. If N_{A0} is the number of moles of A initially in the reactor. then the total number of moles of A that have reacted after a time t is

$$[N_{A0} \cdot X]$$

[Moles of A reacted (consumed)] =

[Moles of A fed].[Moles of A reacted/Moles of A fed]

[mole of A reacted (consumed)] = $[N_{A0}].[X]$

Now, the number of moles of A that remain in the reactor after a time t , N_A can be expressed in terms of N_{A0} and X :

$$N_A = N_{A0} - N_{A0} \cdot X$$

The number of moles of A in the reactor after a conversion X has been achieved is :

$$N_A = N_{A0} - N_{A0} \cdot X = N_{A0}(1 - X)$$

When no spatial variations in reaction rate exist, the mole balance on species A for a batch system is given by

$$dN_a/dt = r_a \cdot V$$

This equation is valid whether or not the reactor volume is constant. In the general reaction. Reactant A is disappearing: therefore, we multiply both sides of Equation to obtain the mole balance for the hatch reactor in the form:

$$-dN_a/dt = -r_a \cdot V$$

For batch reactors, we are interested in determining how long to leave the reactants in the reactor to achieve a certain conversion X. To determine this length of time, we write the mole balance in terms of conversion by differentiating Equation with respect to time, remembering that N_{A0} is the number of moles of A initially present and is therefore a constant with respect to time.

$$dN_a/dt = 0 - (N_{A0} \cdot dX/dt)$$

Combining the above with Equation yields

$$(dX/dt) \cdot N_{A0} = -r_a \cdot V$$

For a batch reactor, the design equation in differential form is :

$$(dX/dt) \cdot N_{A0} = -r_a \cdot V$$

We call Equation the differential form of the design equation for batch reactor because we have written the mole balance in terms of conversion, the differential forms of the batch reactor mole balances are often used in the interpretation of reaction rate data and for reactors with heat effects, respectively. Batch reactors are frequently used in industry for both gas-phase and liquid-phase reactions. Liquid-phase reactions are frequently carried out in batch reactors when small-scale production is desired or operating difficulties, rule out the use of continuous flow systems. For a constant-volume batch reactor $V = V_0$ Equation can be

$$1/V_0 \cdot dN_A/dt = d(N_A/V_0)/dt = dC_A/dt$$

As previously mentioned, the differential form of the mole balance, Equation . is used for analyzing rate data in a batch reactor.

The reaction order and the rate law :-

The Reaction Order and the Rate Law In the chemical reactions considered in the following paragraphs, we take as the basis of

calculation a species A, which is one of the reactants that is disappearing as a result of the reaction. The limiting reactant is usually chosen as our basis for calculation. The rate of disappearance of A – r_A depends on temperature and composition. For many reactions it can be written as the product of a reaction, reaction rate constant A k and a function of the concentrations of the various species involved in the reaction:

$$R = [k(T)][f_n(C_A, C_B, \dots)]$$

The algebraic equation that relates A – r to the species concentrations is called the kinetic expression or rate law. The specific rate of reaction (also called the rate constant k_A , like the reaction rate $-r_A$ always refers to a particular species in the reaction and normally should be subscripted with respect to that species.

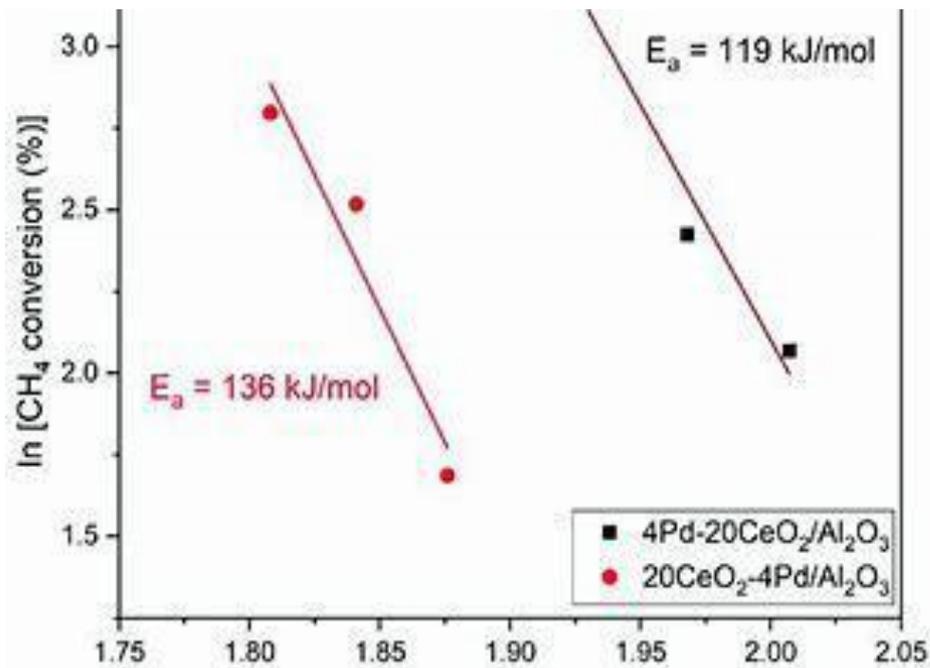
The reaction rate constant The reaction rate constant k is not truly a constant: it is merely independent of the concentrations of the species involved in the reaction. The quantity k is referred to as either the specific reaction rate or the rate constant. It is almost always strongly dependent on temperature. It depends on whether or not a catalyst is present, and in gas-phase reactions, it may be a function of total pressure. In liquid systems it can also be a function of other parameters, such as ionic strength and choice of solvent. These other variables normally exhibit much less effect on the specific reaction rate than temperature does with the exception of supercritical solvents, such as super critical water. Consequently, for the purposes of the material presented here, it will be assumed that k_A , depends only on temperature. This assumption is valid in more laboratory and industrial reactions and seems to work quite well. It was the great Swedish chemist Arrhenius who first suggested that the temperature dependence of the specific reaction rate, k_A , could be correlated by an equation of the type

$$k [T] = Ae^{-E/RT}$$

Where A = frequency factor E = activation energy. J/mol or cal/mol R = gas constant = 8.314 J/mol.K = 1.987 cal/mol.K T= absolute temperature, K Postulation of the Arrhenius equation, is determined experimentally calculation of the by carrying out the reaction at several different temperatures. After taking the natural logarithm we obtain:

$$\ln k_A = \ln A - E/RT$$

and see that the activation energy can be found from a plot of $\ln k$ as a function of $(1/T)$

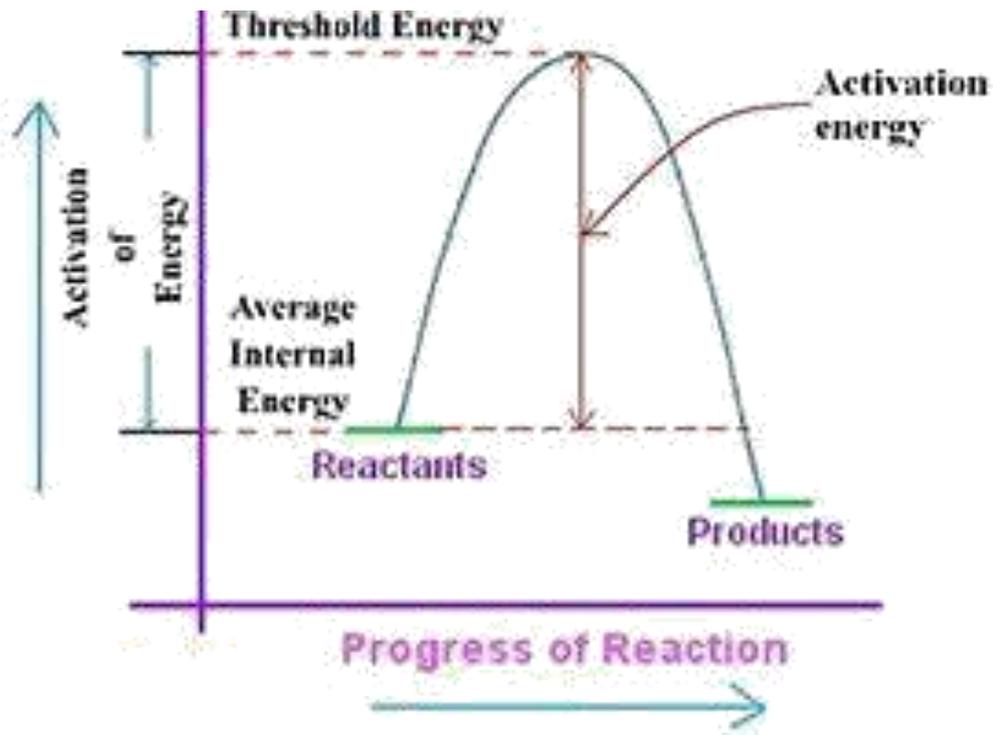


Examples of reaction rate:- laws Zero Order Reaction:

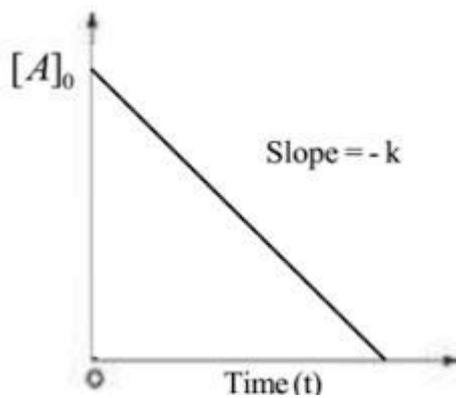
o Rate law: $-r_A = k = dC_A/dt$

o Separate and integrate:

$$\int -dC_A = \int k dt$$



$$C_{A0} - C_A = kt$$



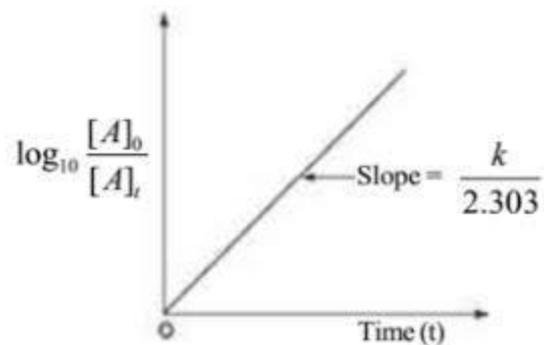
First Order Reaction:



o Rate law: $-r_A = kC_A = dC_A/dt$ o Separate and integrate:

$$\int -dC_A/C_A = \int k dt$$

$$\ln(C_{A0}/C_A) = kt$$



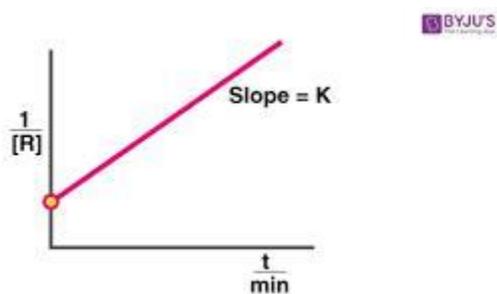
Second Order Reaction: 1. $2A \rightarrow \text{Product}$, $A + B \rightarrow \text{Products}$ $C_{A0} = C_{B0}$

o Rate law: $-r_A = kC_A^2 = dC_A/dt$

Separate and integrate :

in term of conversion :

Where $C_A = C_{A0} - X_A$, $kC_A t X_{A0}$



$A + B \rightarrow \text{Products}$

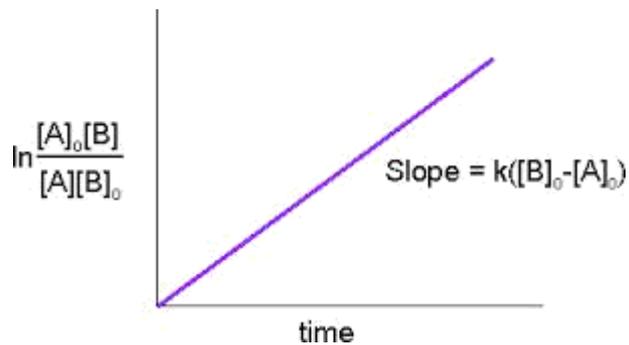
$$C_{A0} \neq C_{B0}$$

o Rate law:

$$-r_a = -dC_a/dt = kC_a C_b$$

o Separate and integrate :

$$\ln(M - x_a)/(1 - x_a) = \ln(C_B C_{A0})/(C_{B0} C_A) = (C_{B0} - C_{A0})Kt$$



Collection and analysis of rate data :-

Assume that the rate law is of the form

$$-r_a = K_a C_a^\alpha$$

Batch reactors are used primarily to determine rate law parameters for homogeneous reactions. This determination is usually achieved by measuring concentration as a function of time and then using either the differential, integral method of data analysis to determine the reaction order, α , and specific reaction rate constant, K_a .

However, by utilizing the method of excess, it is also possible to determine the relationship between $-r_a$ and the concentration of other reactant. That is for the irreversible reaction below Equation :



$$-r_a = K_a C_a^a C_b^b$$

where a and b are both unknown, the reaction could first be run in an excess of B so that C_b remains essentially unchanged during the course of the reaction and

$$-r_a = K_a C_a^a C_b^b = K' C_a^a$$

After determining a , the reaction is carried out in an excess of A , or equal molar to get overall reaction order .

$$-r_a = K C_a^a C_b^b = K'' C_a^a$$

Chapter 3

Differential method of analysis

To outline the procedure used in the differential method of analysis, we consider a reaction carried out isothermally in a constant-volume

batch reactor and the concentration recorded as a function of time. By combining (the mole balance with the rate law given by

$$-dC_a/dt = K_a C_a^{\alpha}$$

After taking the natural logarithm of both sides of Equation

$$\ln(-dC_a/dt) = \ln(K_a) + \alpha \ln(C_a)$$

Numerical method:-

Numerical differentiation formulas can be used when the data points in the independent variable are equally spaced. Such as $t_1 - t_0 = t_2 - t_1 = \Delta t$.

| | | | | |
|------------------------------------|-----------------------|-----------------------|-----------------------|-----------------------|
| Time(sec) | t₀ | t₁ | t₂ | t₃ |
| Concentration (mol/lit) | C_{A0} | C_{A1} | C_{A2} | C_{A3} |

Polynomial fit:-

Another technique to differentiate the data is to fit the concentration time data to an nth-order polynomial:

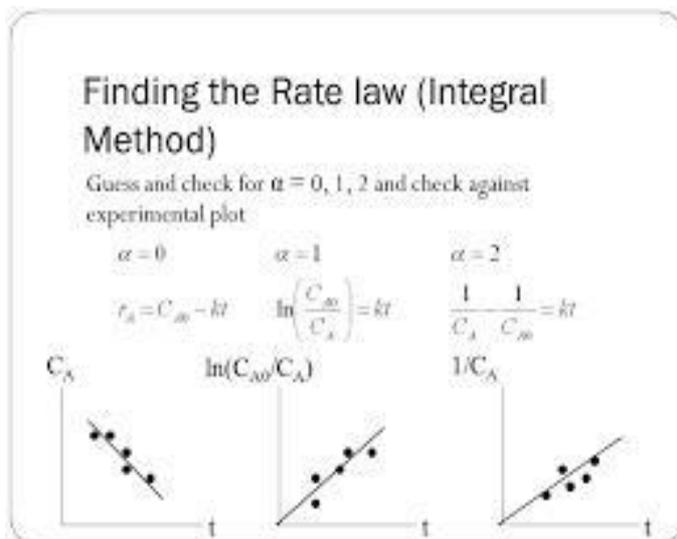
$$C_a = a_0 + a_1 t + a_2 t^2 + \dots$$

$$dC_a/dt = a_1 + 2a_2 t + 3a_3 t^2$$

Many personal computer software packages contain programs that will calculate the best values for the constants a_i . One has only to enter the concentration time data and choose the order of the polynomial. After determining the constants a_1 , one has only to differentiate.

Integral method of analysis:-

To determine the reaction order by the integral method, we guess the reaction order and integrate the differential equation used to model the batch system. If the order we assume is correct, the appropriate plot (determined from this integration) of the concentration-time data should be linear. The integral method is used most often when the reaction order is known and it is desired to evaluate specific reaction rate constants at different temperatures to determine order and the activation energy. In the integral method of analysis of rate data, we are looking for the appropriate function of concentration corresponding to a particular rate law that is linear with time. You should be thoroughly familiar with the methods of obtaining these linear plots for reactions of zero, first, and second order. For the reaction:



Comparison between differential and integral methods.

Integral Method:-

- Easy to use and is recommended for testing specific mechanism

- Require small amount of data
- Involves trial and error
- Cannot be used for fractional orders
- Very accurate

Differential Method:-

- Useful in complicated cases
- Require large and more accurate data
- No trial and error
- Can be used for fractional orders
- Less accurate.

Chapter 4

Objective:-

To study the saponification reaction in ideal batch reactor and find the kinetic parameters using MATLAB and to study about batch reactor.

Case Study:-

Studying the saponification reaction of ethyl acetate with sodium hydroxide in ideal batch reactor at isothermal condition.

Material Required and methods:-

Materials Chemicals:-

1. Phenolphthalein Use as indicator is added to the acid in the E-flask . Causes the solutions to change color when the acid is neutralized.
2. Hydrochloric Acid (HCl) Properties: Liquid, Concentration 32 %, M.W 36.46,Wt.per ml at C 0 20 equal 1.189 g/ml
3. Sodium Hydroxide (NaOH) Properties: Solid Pellets, M.W 40. 00
4. Ethyl Acetate($\text{CH}_3\text{COOC}_2\text{H}_5$) Properties: liquid, Concentration 99 %, M.W 88.11, Wt.per ml at 20 0 C equal 0.902 g/ml
5. Distillated water was Prepared in unit operation lab.

Chapter 5

Procedure:

1. Prepare a solution of N/10 ethyl acetate by mixing appropriate amount of ethyl acetate in 1L of solution
2. Prepare a solution of N/10 NaOH by dissolving 4gm in 1L Solution
3. . Prepare a solution of N/10 HCl and N/10 NaOH (4gm NaOH in 1L solution) for the titration
4. use phenolphthalein as indicator
5. Take 5 no of 250ml conical flasks and put 20ml N/10 HCl in each Flask
6. Take N/10 NaOH in the burette
7. Adjust the temperature of water bath at required temperature
8. Take 400 ml each of N/10 $\text{CH}_3\text{COOC}_2\text{H}_5$ and N/10 NAOH in two seperate flasks and keep them in the water bath for about 15 min.
9. Transfer the solution in the batch reactor start immediately the mixture and the stop watch.
10. At regular intervals of 5min withdraw 10ml of reaction mixture and put it in the marked flask
containing N/10 HCl. take al least 5 sample at regular intervals of time
11. Titrate the excess N/10 HCl in each flask using N/10 NaOH from burette and phenolphthalein as indicator.
12. Record the reaction temperature.



Observation and Experimental values:-at 318 k at 0.1 N

| Time(min) | Titre value in ml |
|-----------|-------------------|
| 0 | 16.7 |
| 5 | 17.0 |
| 10 | 17.3 |
| 15 | 17.5 |
| 20 | 17.8 |
| 25 | 18.1 |
| 30 | 18.4 |

at 328 k at 0.1 N

| Time(min) | Titre value in ml |
|-----------|-------------------|
| 0 | 17.4 |
| 5 | 17.7 |
| 10 | 18.0 |
| 15 | 18.2 |
| 20 | 18.6 |
| 25 | 18.8 |
| 30 | 19.1 |

| | |
|--|--|
| | |
|--|--|

At 338k at 0.1N

| Time(min) | Titre value in ml |
|-----------|-------------------|
| 0 | 17.5 |
| 5 | 17.8 |
| 10 | 18.2 |
| 15 | 18.3 |
| 20 | 18.7 |
| 25 | 18.9 |
| 30 | 19.2 |

At 343k at 0.1N

| Time(min) | Titre value in ml |
|-----------|-------------------|
| 0 | 17.5 |
| 5 | 17.9 |
| 10 | 18.3 |
| 15 | 18.5 |
| 20 | 18.9 |
| 25 | 19.1 |
| 30 | 19.5 |

At 328 k 0.1N ethyl acetate and 0.2 N Naoh

| Time(min) | Titre value in ml |
|-----------|-------------------|
| 0 | 13.0 |
| 5 | 13.8 |
| 10 | 14.4 |
| 15 | 15.2 |
| 20 | 15.5 |
| 25 | 16.1 |
| 30 | 16.5 |

At 328 k 0.1N ethyl acetate and 0.5 N Naoh

| Time(min) | Titre value in ml |
|-----------|-------------------|
| 0 | 17.7 |
| 5 | 18.0 |
| 10 | 18.5 |
| 15 | 18.7 |
| 20 | 18.9 |
| 25 | 19.3 |
| 30 | 19.6 |

Chapter 6

MATLAB Code:-

1. Calculating rate constant for varying temperature at fixed initial concentration. Plotting $1/C_a$ versus T graph.

```
function CA=Concentration(titre_value)
CAo=0.05;
Nnaoh=0.1;%strength of naoh
Vsample=10;%volume of sample
tspan1=0:5:30;
HCLr=0.002-(titre_value*Nnaoh*0.001);
CA=(HCLr*1000)/(Vsample);
CA= [CAo;CA]
scatter(tspan1,1./CA)
|
%CURVE FITTING
p=polyfit(tspan1,1./CA,1)

%fit model to data
ydata=polyval(p,tspan1);

%plot(fitresult,xdata,ydata)
plot(tspan1,ydata)

grid on
xlabel('time')
ylabel('1/CA')
title('1/CA Vs time')
```

```
1 Nnaoh=0.1;%strength of naoh
2 Vhcl=20;%volume of hcl
3 Nhcl=0.1;%strength of hcl;
4 Nea=0.1;%strength of ethyl acetate|
5 tspan= 5:5:25;
6 tspan1=5:5:50;
7 titre_value_1=[17;18.3;20.9;22;23.5];%at 308K
8 titre_value_2=[16.7;17.0;17.3;17.5;17.8;18.1;18.4;18.8;19.5;19.9];%at 318k
9 titre_value_3=[17.4;17.7;18.0;18.2;18.6;18.8;19.1;19.5;20.3;20.7];%at 328k
10 titre_value_4=[17.5;17.8;18.2;18.3;18.7;18.9;19.2;19.7;20.5;20.9];%at 338k
11 titre_value_5=[17.5;17.9;18.3;18.5;18.9;19.1;19.5;20.2;20.7;21.2];%at 343k
12 %CA1=Concentration(titre_value_1);
13 titre_value_2=titre_value_2(1:6,1);
14 titre_value_3=titre_value_3(1:6,1);
15 titre_value_4=titre_value_4(1:6,1);
16 titre_value_5=titre_value_5(1:6,1);
17
18 CA2=Concentration(titre_value_2);
19 hold on
20 CA3=Concentration(titre_value_3);
21 CA4=Concentration(titre_value_4);
22 CA5=Concentration(titre_value_5);
23
24
25
26
```

2. Calculating Activation Energy for given reaction using Arrhenius Equation and then plotting Arrhenius plot.

```
K=[0.9633;1.9144;2.1424;2.8157];
T=[318;328;338;343];
scatter(T,K)
lnk=log(K);
scatter(1./T,lnk);
%CURVE FITTING
p=polyfit(1./T,lnk,1)

%fit model to data
ydata=polyval(p,1./T);

%plot(fitresult,xdata,ydata)
plot(1./T,ydata)
grid on
xlabel('1/T')
ylabel('lnk')
title('Arrhenius plot')
R=8.314;
Ea=-1*R*p(1)
A=exp(p(2))
```

Value of activation energy E_a in joules is given

$$E_a = 3.5755e+04$$

3. Calculating Reaction rate constant for different initial concentration at 328K.

```

1 function CA=concen(titre_value,M,CAo)
2   Nnaoh=0.1;%strength of naoh
3   Vsample=10;%volume of sample
4   Vhcl=20;%volume of hcl
5   Nhcl=0.1;%strength of hcl;
6   tspan1=5:5:30;
7   CA=((Vhcl*Nhcl)-(titre_value*Nnaoh))/(Vsample);
8   XA=1-CA/CAo
9   Ydata=log((M-XA)/(M*(1-XA)));
0   Xdata=tspan1;
1   %CURVE FITTING
2   p=polyfit(tspan1,Ydata,1)
3
4   %fit model to data
5   y=polyval(p,tspan1);
6
7   %plot(fitresult,xdata,ydata)
8   plot(tspan1,y)
9
0   scatter(Xdata,Ydata)
1   grid
2   xlabel('time')
3   ylabel('ln((M-XA)/ M(1-XA))')
4   title('ln((M-XA)/ M(1-XA)) vs time')

```

```

Nnaoh=0.1;%strength of naoh
Vhcl=20;%volume of hcl
Nhcl=0.1;%strength of hcl;
Nea=0.1;%strength of ethyl acetate
tspan= 5:5:25;
tspan1=5:5:50;
CAo=[0.2;0.5];
Mratio=[5;2];
titrevalue_1=[13.0;13.8;14.4;15.2;15.5;16.1;16.5;16.9;17.2;18.0];% at
titrevalue_2=[17.7;18.0;18.5;18.7;18.9;19.3;19.6;19.7;19.8;20.2];% at
titrevalue_1=titrevalue_1(1:6,1);
titrevalue_2=titrevalue_2(1:6,1);
CA1=concen(titrevalue_1,Mratio(1),CAo(1));
hold on
CA2=concen(titrevalue_2,Mratio(2),CAo(2));

```

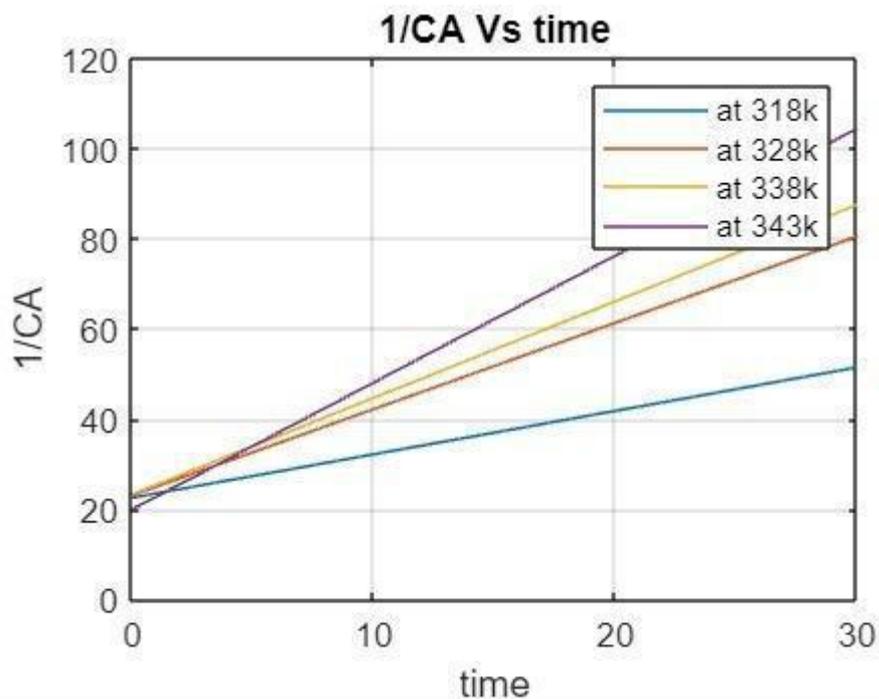
4. Evaluating concentration profile of NaOH with respect to time at different temperature.

```
function dcdt=batchreactorfun(t,c)
k=[0.9633;1.9144;2.1424;2.8157];
dcdt=[-k(1)*c(1)^2;-k(2)*c(2)^2;-k(3)*c(3)^2;-k(4)*c(4)^2]

co=[0.05;0.05;0.05;0.05]
tspan=5:2:30;
[t,c]=ode45('batchreactorfun',tspan,co)
plot(t,c)
grid on
xlabel('time')
ylabel('concentration')
title('concentration vs time')
legend('at 318k','at 328k','at 338k','at 343k')
```

Result and Discussion:-

Graph1



The plot is between $1/C_a$ versus t . According to the equation $1/C_a = Kt + 1/C_{a0}$. The slope of the graph is the value of rate constant K at different temperature. As, the figure depicts the value of rate constant K at higher temperature is more than that at lower temperature.

The obtained value of K in $\text{conc}^{-1}\text{min}^{-1}$ at different temperature is listed below.

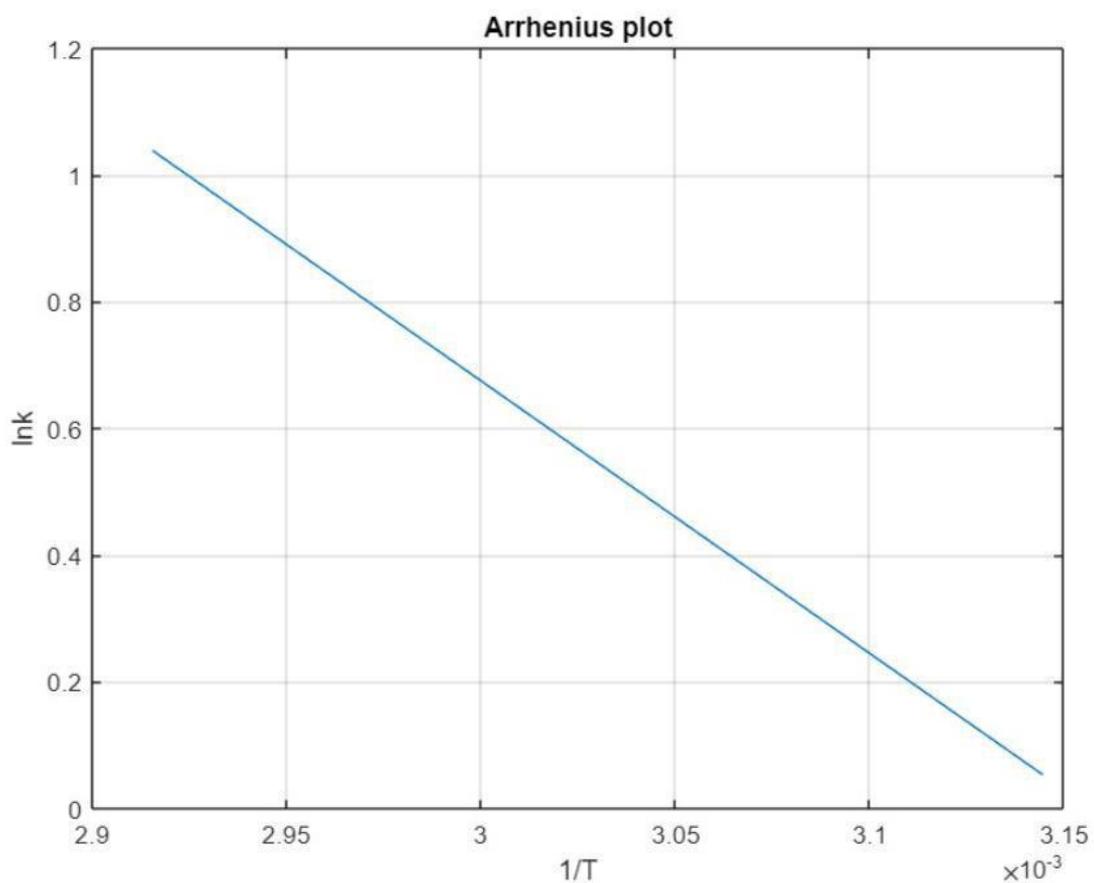
$K=0.9633$ at 318 k

$K=1.9144$ at 318 k

$K=2.1424$ at 318 k

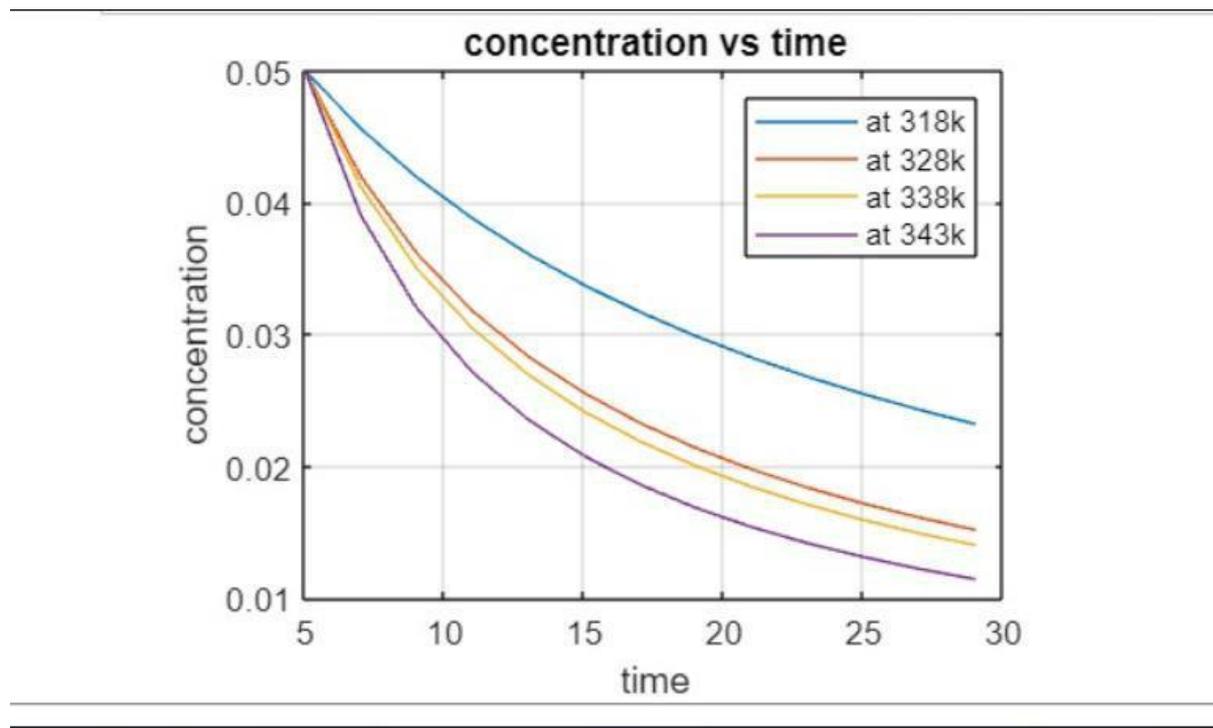
$K=2.8157$ at 318 k

Graph 2



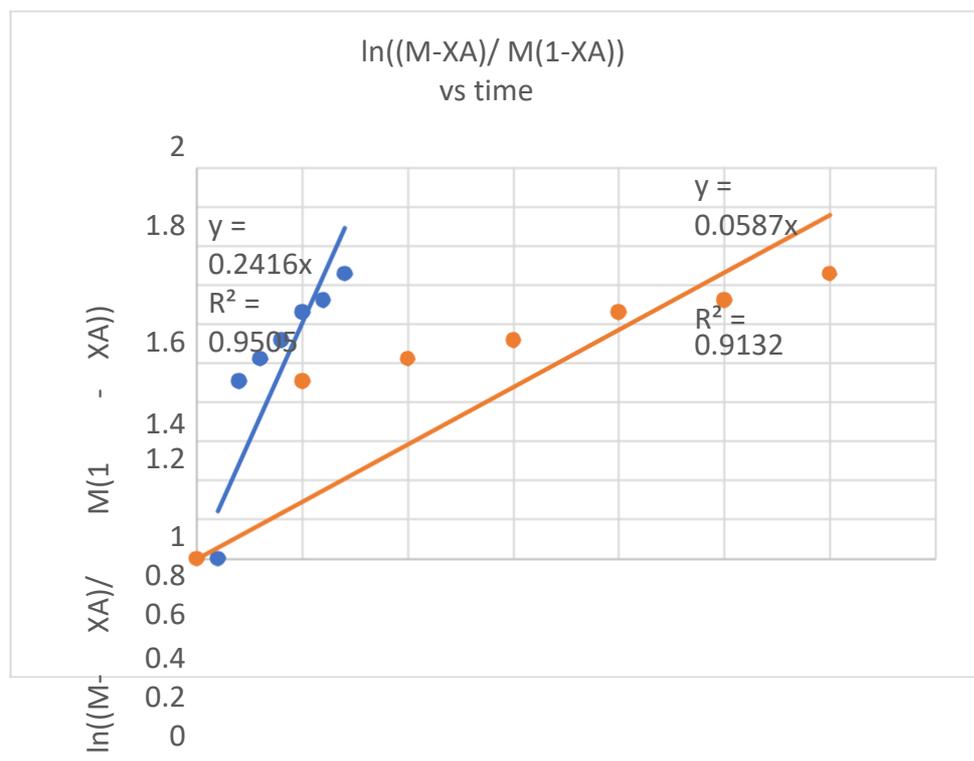
The plot is between $\ln k$ versus $1/T$. According to the equation $\ln k = -E_a/RT + \ln A$. The slope of the graph is the value of $-E_a/R$ for saponification reaction. The value of activation energy is 35.77 kJ

Graph 3



The plot is between concentration versus t according to the equation $1/C_a = Kt + 1/C_{a0}$ at different temperatures

Graph 4



0 5 10 15 20 25 30 35
time

Chapter 7

References:-

1. Fogler, S. H.; "Elements of Chemical Reaction Engineering," Prentice Hall, 4rd Edition (2006).
2. <http://api.uofk.edu:8080/api/core/bitstreams/308421e6-2174-4f92-ad53-c1108cdeab0c/content>
3. <https://modelingandcontrol.com/2011/05/applications-batch-chemical-reactor-control-2/>
4. <https://www.sciencegate.app/keyword/35979>
5. https://www.academia.edu/Documents/in/Batch_Reactor