

Review On Kinetics of High Temperature Esterification and Its Process Design

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Abstract: Esterification reactions are vital in industrial applications, particularly in the production of biodiesel, pharmaceuticals, and specialty chemicals. This study investigates the kinetics of high-temperature esterification reactions, focusing on the thermodynamic and kinetic parameters that influence reaction rates and product yield. The ester and water are yielded by the reaction between an alcohol and a carboxylic acid., with the reaction rate dependent on temperature, pressure, catalyst type, and reactant concentrations. A mathematical model was developed to describe the reaction kinetics, incorporating both the Arrhenius equation for temperature dependence and a Langmuir-Hinshelwood mechanism for catalytic reactions. Experimental data from high-temperature esterification experiments were used to determine the activation energy and rate constants, providing a comprehensive understanding of the process dynamics. The results indicated that the reaction rate increased significantly with temperature, following first-order kinetics with respect to both reactants under the studied conditions. Furthermore, process design considerations were explored, including the selection of optimal reactor types, temperature profiles, and reactor sizing. The influence of equilibrium constraints and separation processes, particularly water removal, was also analyzed. The findings highlight the importance of maintaining a high temperature to achieve desirable reaction rates while addressing practical limitations related to catalyst deactivation and heat

transfer. This research offers valuable insights into the optimization of high-temperature esterification processes, contributing to the efficient design and scaling of industrial reactors for ester production. The kinetic model and process design guidelines established in this study can be applied to improve the performance and economic viability of esterification-based chemical manufacturing.

Keywords: Arrhenius equation, Langmuir-Hinshelwood mechanism, activation energy, rate constants, process design, catalyst deactivation

1. INTRODUCTION

Polyester polyol is saturated and has terminal hydroxyl groups, and is used in polyurethane production. Both rigid and flexible polyurethanes are made from polyester polyols. Polyester polyols are more expensive than polyether polyols and are also more viscous at the same temperature. Polyester polyols will produce polyurethane with more heat stability than polyether polyols. Polyester polyol has wide application for coating adhesives and elastomers. Polyester polyols are synthesized via an esterification reaction step. Usually, the esterification is completed at temperature above 200°C with nitrogen or CO₂ as blanket or directly vacuum is used to remove water and to reach the expected conversion and It is expected that resulting polyester will have an acid value less than 1 mg KOH/g [1-5]

An ester is formed as a reaction product when two reactants, typically an alcohol and an acid, undergo esterification. Organic chemistry and biological materials often contain ester. Fischer-esterification is a type of esterification that involves refluxing a carboxylic acid and an alcohol, generally a diol, in the presence of an acid catalyst. Sulfuric acid, Tosylic acid, and Lewis acids such as Scandium (III) Triflate are used as catalysts for Fischer esterification. The

reaction was first described by Emil Fischer and Arthur Speier in 1895. The nucleophilic substitution of an alcohol on a carbonyl carbon is an example of Fischer esterification

A dicarboxylic acid is an organic compound containing two or more carboxylic functional groups (-COOH). The general molecular formula for dicarboxylic acid can be written as HO₂C-R-CO₂H, where R can be aliphatic or aromatic. Polymers such as polyamide and polyesters are prepared using dicarboxylic acids. Adipic acid can be abbreviated to diacid. Industrially, nylon is produced by the oxidation of cyclohexanol or cyclohexane. Mainly for the production of Nylon -6,6 [6-8]

A glycol is a chemical compound containing two hydroxyl groups (-OH groups). Many subcategories have been identified for this pairing of functional groups. Polyurethanes and alkanol resins are produced by the dominant reactions of diols. Polyesters and polyurethanes are formed by polymerization reactions using diol monomers such as ethylene glycol. [9-10]



Where,

Either an alkyl or aryl group is R or R'.

The conversion of a reaction is improved by using alcohol in large excess or using a dehydrating agent or removal of water by physical means or by addition of catalyst. Kinetics of reaction depends on condition inside the reactor. A chemical reaction has the tendency to approach equilibrium. Reaction rate depends on concentration, temperature, pressure and time of reaction for a batch reactor.

The present work is based on establishing and developing the kinetics of the reaction, followed by optimizing the process parameters for better throughput of the reactor. The second chapter reviews the synthesis of polyester polyol under different process conditions along with the design of the required equipment and the parameters of the same. The third chapter deals with the detailed study on the synthesis of polyester polyols followed by the kinetic study of

the performed reaction. Further, this chapter discusses the process as well mechanical design of the unit processes and unit operations used for the successful synthesis of polyester polyols. The fourth chapter explains the final results and their values followed by their optimization wherever required. Finally, the work ends with concluding words [11-14].

2. LITERATURE REVIEW

2.1 Esterification

Esters can be synthesized through several routes. The direct esterification of carboxylic acids with alcohols in the presence of a mineral acid catalyst is the most widely used method [15-17].



Where

Either an alkyl or aryl group is R or R'.

Esters formed from simple hydrocarbon groups are colourless, volatile liquids with pleasant aromas, and fragrance is given to flowers and fruits by them. These unique features are made possible by esterification, which is a very slow and highly reversible reaction. The equilibrium determines the limiting conversion of the reactants. The following methods can improve the equilibrium constant or the conversion of a reversible reaction: [Beula, 2015][1]

- Alcohol is used in large excess
- A dehydrating agent is used
- Water is removed
- Addition of a catalyst

This esterification reaction proceeds with a reaction constant K, which is defined as

$$K = \frac{[\text{polyester polyol}][H_2O]^{2n}}{[\text{diacid}]^n[\text{diol}]^{n+x}} \quad (1)$$

Where,

n – Moles of diacid

x – Excess of diol (in terms of mole fraction)

[] – concentration of the reactant or product mentioned within it.

It can be clearly concluded from this equation that the forward rate of reaction for the synthesis of polyester polyol is influenced by the presence of water in the equilibrium with the reactants and the polymer. The removal of water in the latter part of the reaction process is essential for the building up of the required molecular weight. The esterification reaction is influenced by factors such as reaction temperature, agitation, and the quality and flow rate of the inert gas used. An inert gas, such as nitrogen, is used to prevent oxidation and help remove the water formed during the polycondensation reaction.

The residual water is removed by increasing the inert gas rate at the final stages of the polyesterification. Reduced pressure can facilitate the removal of water at this stage

2.2 Adipic Acid

Adipic acid, the most widely used dicarboxylic acid in the industry, is a precursor used in the production of nylon. It is generally produced from Cyclohexene. [18-20]

2.2.1 Applications of Adipic Acid

Precursor for Nylon

Nylon is synthesized from adipic acid, as we mentioned. Industrial chemists make nylon by taking adipic acid and reacting it with hexamethylene diamine. Nylon itself finds use in many application including fibres, plastics, filaments and food packing materials.

Medicinal Use

Although adipic acid itself doesn't find use as a therapeutic agent, it has still found use in the medicinal and pharmaceutical industries. Adipic acid has been incorporated into drug tablets in order to help with the controlled release of both acid and basic drug compounds.

In food

Adipic acid find use in the in food industries as both flavouring and gelling aid for things like jelly. Have you ever had to take an antacid tablet? Adipic acid is sometimes used in these tablets to give them that tort flavour you taste when you take them. Figure 1 Global Consumption of Adipic Acid shows that

2.2.2 Global consumption of Adipic Acid

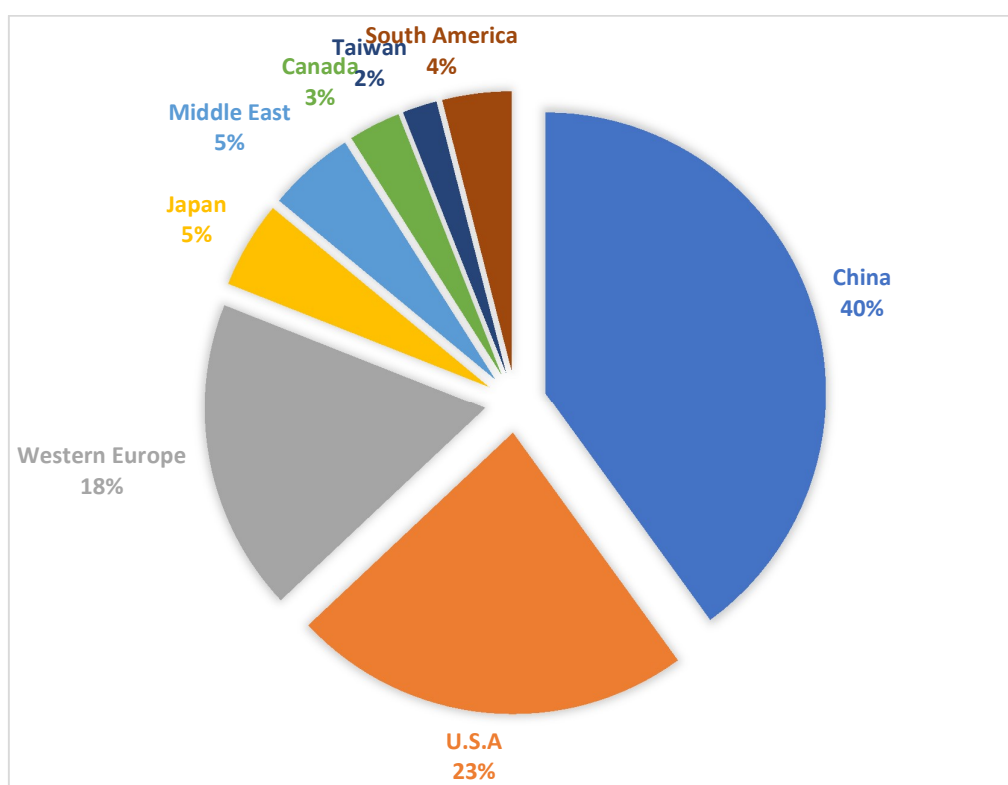


Figure 1: Global Consumption of Adipic Acid

2.3 Neopentyl Glycol

Neopentyl glycol (IUPAC name: 2,2-dimethylpropane-1,3-diol) is an organic chemical compound. Polyesters, paint, lubricants, and plasticizers are synthesized from neopentyl glycol. The use of [ingredient] enhances the stability of polyesters towards heat, light, and water. Synthetic lubricating esters with reduced potential for oxidation or hydrolysis are produced by esterification reaction with fatty or carboxylic acids Kumar et al., [Kumar and Gupta 2024].

2.3.1 Applications of Neopentyl Glycol

- i. Base resins for coatings
- ii. Hydraulic fluids
- iii. Synthetic lubricant oils
- iv. Greases
- v. Metal-working fluids
- vi. Pesticide
- vii. Plasticizers

2.3.2 Global Consumption of Neopentyl Glycol

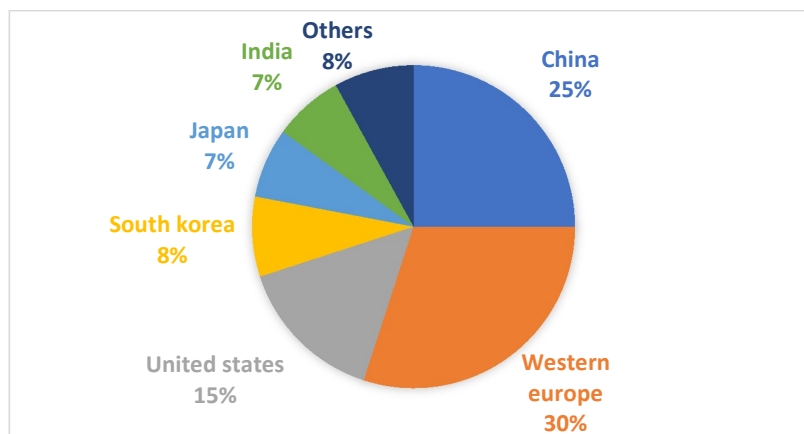


Figure Error! No text of specified style in document.: Global Consumption of Neopentyl Glycol

2.4 Catalyst

The synthesis of polyester polyol is significantly influenced by catalysts. Researchers have studied all the possible catalysts that can be used for the synthesis of the polyester polyol. Several catalysts used by various researchers for the synthesis of different polyester polyols with their concentration has been mentioned in Table 2.

In addition to this N. Jacquel et. al. [5] studied the efficiency of different transesterification catalysts for the synthesis of poly(butylene succinate). The catalyst in consideration was either based on organometals (Titanium, Zirconium, Tin) or were some metal oxides of Germanium and Antimony. In this system no solvent was employed, rather the polymerization was carried out by two-step melt polycondensation. OH/COOH ratio of 1.05 was incorporated for this system. A temperature of 225°C was attained. The completion of the reaction for all the systems (involving different catalysts) was determined when the stirrer attained a specific torque. The reaction time was noted for different catalysts and for different concentrations.

The transesterification step was studied when titanium catalyst was added before and during. The transesterification reaction completion was delayed when the catalyst was added before

the step, unlike when it was added during the step. The poisoning of the catalyst during the esterification process is a possible reason for its behavior. Water, generated as a by-product, is the source of the poisoning.

Next, study [4] determined the efficiency of the catalyst by the torque method, as mentioned before. The study revealed that the Ti-based catalyst was the most effective as shown in Fig. 3. The same rate of reaction was produced by Zr- & Sn-based catalyst but at higher concentrations. Ge- & Sb-based catalyst showed a decreased rate of reaction at higher concentrations.

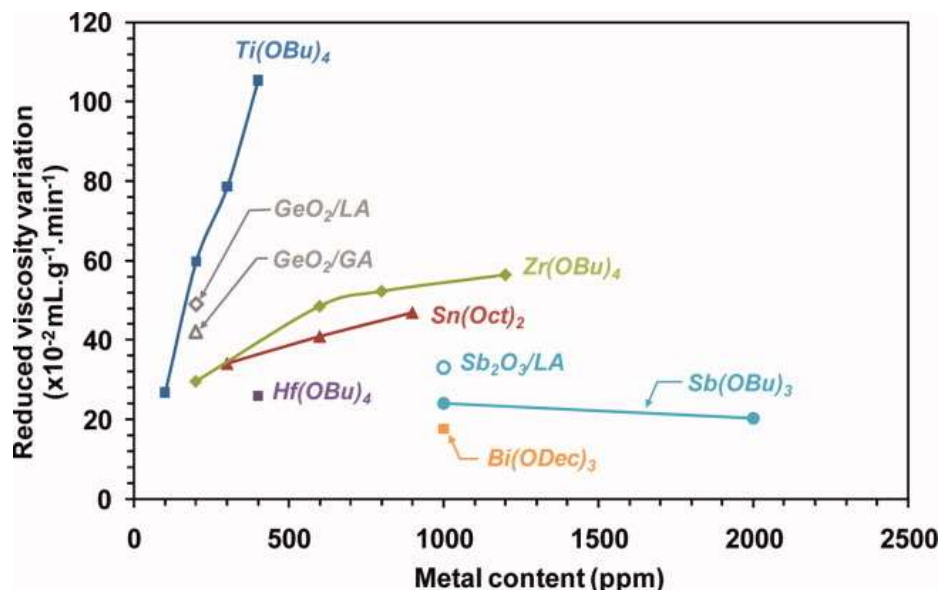


Figure 3: Effectiveness of Different Catalysts Used for Polyester Polyol Synthesis

The effect of the catalyst was studied by the researchers on the storage of poly (butylene succinate). The viscosity change over time was taken as a measure of the degradation of poly(butylene-succinate). The study resulted in the conclusion that the poly(butylene-

succinate) synthesized using Ti-based catalyst had faster degradation over time, as compared to Sn-based catalyst [4].

Out of all the studies made, it was first noted to add the catalyst during the transesterification step Bobba et al., [6]. Secondly, even if the Ti-based catalyst proved to be better for the synthesis; but considering the shelf-life, it was preferred to use Sn-based catalyst for the synthesis of poly (butylene succinate). Thus, commercially available Butyl Stannoic acid was employed for the process. As per the above study, an optimum of 300 ppm of catalyst based on diacid was incorporated.

Table 1: Properties Of Butyl Stannoic Acid

Sr. No.	Properties	Specifications
1	Formula	BuSnOOH
2	% Sn	56.8
3	Molecular Weight	208.8

2.5 Synthesis of Polyester Polyol

For polyol synthesis, it is quite important to determine the OH/COOH ratio. This ratio determines the final molecular weight. For example, for OH/COOH=1, the polyol of very high molecular weight will be formed, while a very low molecular weight polyol would be synthesized if OH/COOH=2. Paul J. Flory, in his study, explained this phenomenon quite effectively [7-8]. Concisely, using this method and applying it, Schrock et. al. explained the calculation of this ratio for predetermined theoretical molecular weight [9] Table 3.

Table 2: Literature Reviewed For Polyester Polyol Synthesis

Author s	Diol		Diacid		Catalyst		Tem p (°C)	Ti me (h r)	Purgi ng Meth od
	Name	Mol	Name	M ol	Name	Conc.			
Pallavi Deshmu kh & Prakash Mahan war [10]	Pentaeryt hritol	0.16- 0.5	Adipic Acid	1	DBTDL	0.05- 0.1%	140 - 190	10	N ₂
	1,6- Hexanedi ol	0.25- 1.0							
	Glycerol	0.2- 0.4	Adipic Acid	1	DBTDL	0.05%	180	7	N ₂
	1,6- Hexanedi ol	0.9							
	1,4- Butanedi ol	0.6- .8	Adipic Acid	1	DBTDL	0.05%	210	7	N ₂
	1,6- Hexanedi ol	0.7							

	Neopentyl glycol	0.6-0.8	Adipic Acid	1	DBTDL	0.05%	210	7	N ₂
	1,6-Hexanediol	0.7							
Lucial Navarro et. al. [11]	Glycerol	0.2-1	Adipic Acid	1	No Catalyst	-	150	16	Vacuum ¹
	Ethylene Glycol	0.25-0.6						-21	
Chin-Tsou Kuo et. al. [3]	1,4-Butanediol	0.99-3.59	Adipic Acid	1	p-toluene sulfonic acid	-	140	6-10	-
	1,6-Hexanediol						-		
	Ethylene Glycol						180		
Radu Bacaloglu et. al. [10]	1,3-Butanediol	1.1	Adipic Acid	1	MBTO, DBTO & MBT		180-215	4-10	N ₂ & Vacuum
V. Tserki		1.1	Adipic Acid	1		0.05%		3-6	

Vacuum was applied during the transesterification step

et. al. [11]	1,4- Butanedi ol		Succini c Acid	1	Titaniu m butoxide		180 - 200		N ₂ & Vacuu m
T. Zorba et. al. [12]	Ethylene Glycol	1.2	Adipic Acid	1	Tetra butyl titanate	0.000 3 mol	190 - 230	-	N ₂ & Vacuu m
	1,4- Butanedi ol								
	1,3- Propaned iol								
D.N. Bikiaris et. al. [13]	Ethylene Glycol	2.2	Dimeth yl terephth alate	1	Zinc Acetate	50 ppm	270	3- 4.5	Ar & Vacuu m
			Trimeth yl Trimell itate		Antimo ny Trioxide	950 ppm			
Huang et. al. [14]	1,4- Butanedi ol	0.98	Adipic Acid	1	Dibutylt in oxide	0.3%	150 - 200	4+	N ₂ & Vacuu m ¹
Sivan Velmath i	1,4- Butanedi ol	1	Succini c Acid	1	1,3- dichloro -1,1,3,3-	0.1 mol	200	5	N ₂

et. al. [15]					tetra- butyl-di- stannox ane				
Masatsu gu Mochiz uki et. al. [16]	1,4- Butanedi ol	1.3	Succini c Acid	1	Titaniu m butoxide	0.001 mol	200	3	N ₂
	Ethylene Glycol				Phospho ric Acid	0.1g			
B. D. Ahn et. al. [17]	1,4- Butanedi ol	1.04- 1.1	Adipic Acid Succini c Acid	1	Titaniu m isopropo xide	-	190 - 220	8- 12	N ₂ & Vacuu m ¹
Momok o Ishii et. al. [18]	1,4- Butanedi ol	1	Succini c Acid	1	Di- stannox ane	0.001- 0.1%	120	24 - 72	-
	Ethylene Glycol								

The chain lengths of the alkyl groups of the diol were found to decrease the activation energies calculated for each system

2.6 Determination of Reaction Kinetics

To understand the reaction kinetics, there are two approaches. Either we calculated the order and rate constant for the reaction under consideration or by pre-knowing the order of reaction, we can calculate the rate constant for the reaction under consideration. In this study both the

techniques have been employed. Their relation and significance are explained further in Chapter 3. In this Chapter we will just review the methodology of reaction kinetic determination.

2.6.1 Differential Method of Analysis of Data

The differential rate equation is evaluated, including the derivative dc/dt , by the differential method of analysis and testing the goodness of fit of the equation with the experiment .

The procedure is as follows:

1) The C_A vs. t data will be plotted, and a smooth curve will be drawn to represent the data.

2) The rates of reaction at these compositions are determined by the slope of the curve.

3) The rate expression for r_A vs. C_A will be found. either by

(a) A particular rate form is picked and tested from $-r_A = kC_A$

(b) A n th order test is being conducted from $-r_A = kC_A^n$

by taking logarithm on both sides

$$\ln (-r_A) = \ln k + n \ln C_A$$

2.7 Draw The Graph of $\ln C_A$ Vs $\ln (-R_a)$ And The Order of the Reaction is determined.

2.7.1 The Integral Method of Analysis of Data is analyzed

Based on the differential method of analysis, a relevant type and order of reaction would be correlated and further using integral method it would be proved that the assumption is correct and thereafter the rate constant would be calculated.

2.8 Design of Batch Reactor

For typical design of batch reactor, following information is required. Depending on the defined parameters and required output, specific inputs can be used.

1. Residence time distribution: Residence time is a measure of how much time the matter spends in it. a small amount of fluid has single residence time, but the more complex system has residence time distribution in a batch reactor the probability that a molecule will react depend only on its residence time

2. Total volume batch reactor
3. Temperature of reaction
4. Working pressure of the reactor
5. The concentration of chemical species
6. Heat /Mass transfer coefficient for the reaction
7. Reaction enthalpies of reactants
8. Phase equilibrium constant of reactants
9. Reaction time of the reaction
10. Reaction rate constant of the reaction
11. Heat and Mass transfer properties of reactants
12. Fluid thermal conductivity of reactants
13. Fluid density of the reactants
14. Superficial velocity of reactants
15. Fluid viscosity of the reactants

2.8.1 Material of Construction for Batch Reactor

Table 3: MOC's

Material	Temperature	Cost / kg
S.S 304	870°C	200/-
INCONEL 625	980°C	800/-
INCONEL 600	1176°C	2700/-
INCONEL 601	1204°C	3000/-
HASTELLOY C22	1204°C	2500/-

As can be seen from the possible and mostly used metals for the construction of batch reactor, stainless steel can withstand high temperature and relatively is cheaper.

2.8.2 Type of Joint for Welding

Several types of joints are available, including butt joints, corner joints, edge joints, lap joints, and tee joints. However, butt joints are commonly used because they are safe and prevent leakage.

2.8.3 Type of Head for Batch Reactor

Elliptical heads are often used for pressure over 10 bar because they resemble an ellipse in cross-section, with a radius varying continuously. A smooth transition is achieved between the dome and the cylindrical part of the vessel

2.8.5 Design of Heat Exchanger

Heat flows from higher temperature to lower temperature, according to the second law of thermodynamics. Heating or cooling is required for solid, liquid, and gas during various operations. Equipment's used for this operation called heat exchanger. General classification

of heat exchangers is shown in the Figure 4. [21-23]

Heat exchangers are classified in various ways

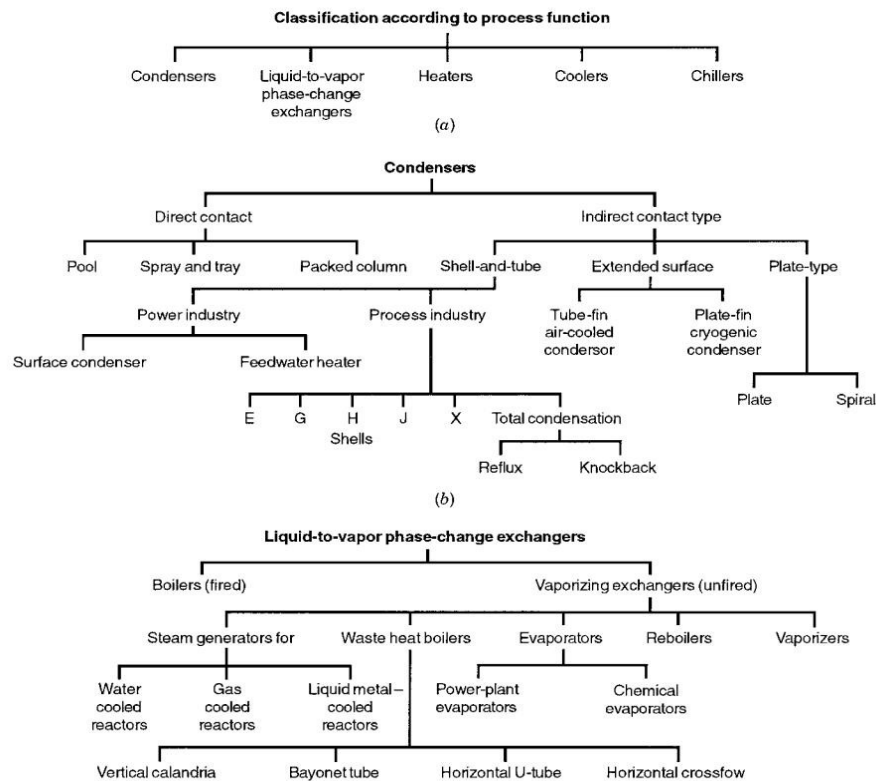


Figure 4: Classification of Heat exchanger

The most commonly used heat exchange equipment among all types of exchangers is shell and tube exchangers. The common types of shell and tube exchangers are identified as:

Fixed Tube-Sheet Exchanger (Non-Removable Tube Bundle)

The simplest and cheapest type of shell and tube exchanger is a fixed tube sheet design. In exchangers of this type, the shell is welded to the tube sheet, and no relative movement is possible between the shell and tube bundle.

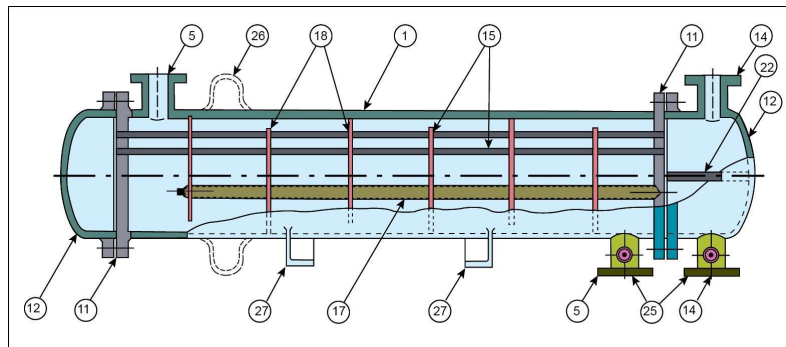


Figure 5: Fixed tube sheet heat exchanger

Removable Tube Bundle

For ease of cleaning and replacement, tube bundles may be removed. Removable tube bundle exchangers can be further categorized by being floating-head and U-tube exchangers.

Floating-Head Exchanger

Maintenance and cleaning of the tube are made easier. The entire tube bundle in a floating head heat exchanger can be easily removed for cleaning and maintenance. While this is not possible in a fixed tube sheet heat exchanger.

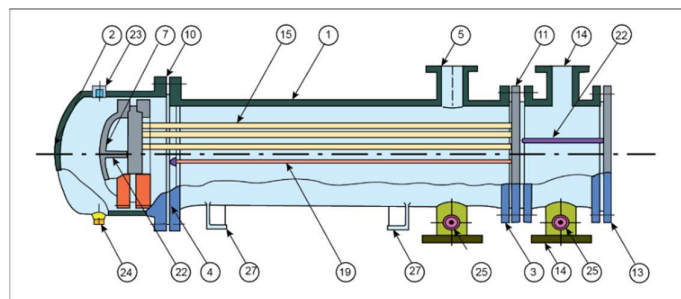


Figure 6: Floating Head Heat Exchangers

U-tube exchanger

The differential thermal expansion or contraction between shell and tube is permitted by U-tube heat exchangers. Therefore, the use of expansion joint is not required in U-tube heat

exchangers. The fixed cost of U-tube heat exchanger is always less than that of floating head heat exchanger for the given duty.

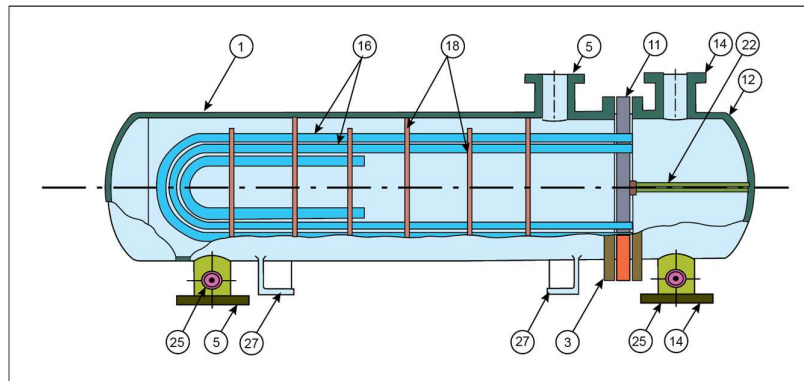


Figure 7: U-tube Heat Exchanger

The selection of this heat exchangers is done based on TEMA standards. The various different types of head closings and the main body have been described in Figure 8.

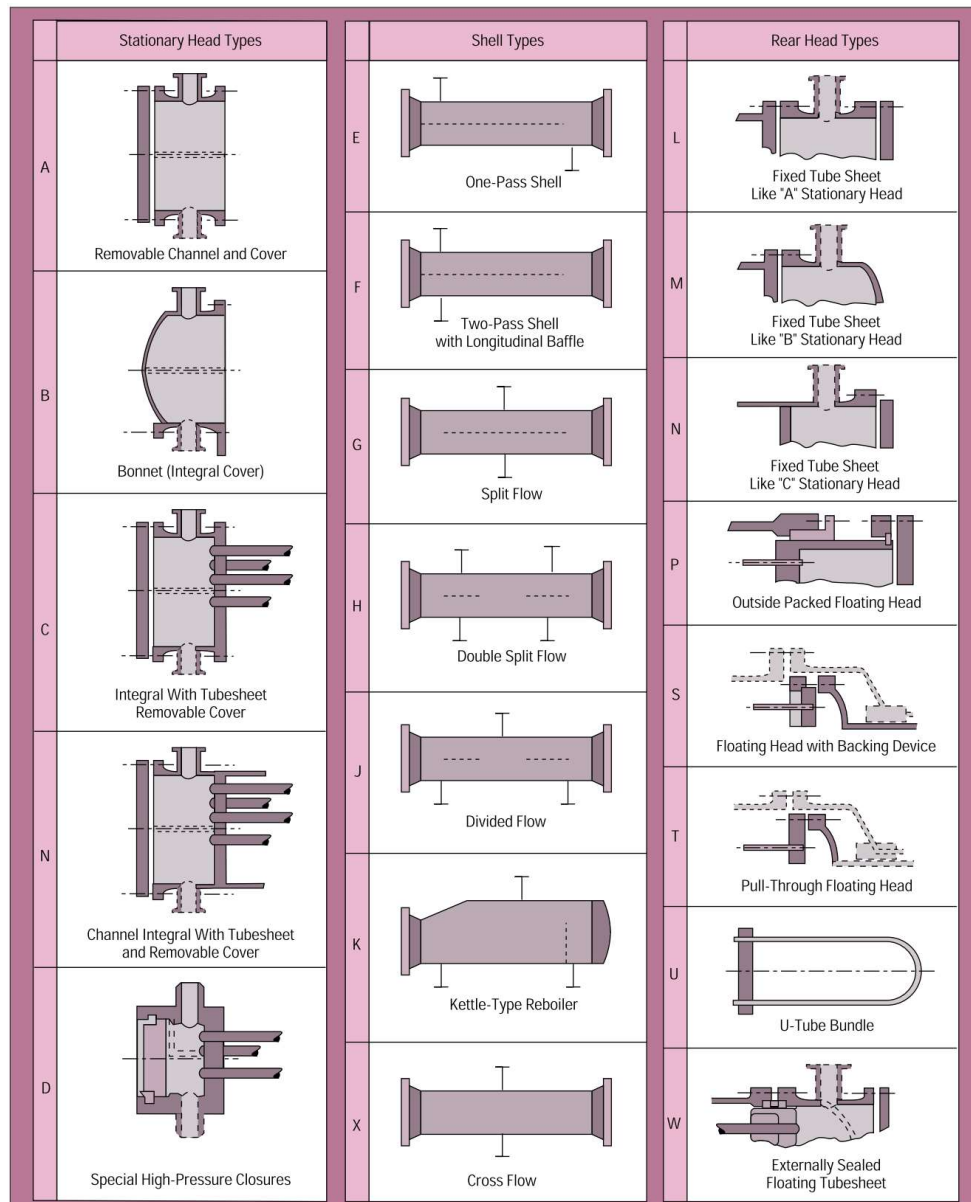


Figure 8: TEMA Standards

2.8.6 Thermal Design Considerations

Calculate heat transfer area, determine number of tubes, decide tube length and diameter, fixed tube layout, number of passes on shell and tube side, type of heat exchanger, tube pitch, types of baffle, baffle cut, tube and shell side pressure drop and overall heat transfer coefficient etc. involve in thermal design of heat exchanger.

Shell

The cost of the shell and tube heat exchanger sensitively changes with the diameter of the shell.

Shell sizes range from 6 in (152 mm) to 60 in (1520 mm), as per the TEMA standard. Standard pipes are available up to 24 in size.

Tube

Tube sizes in shell and tube heat exchangers range from $\frac{1}{4}$ in (6.35 mm) to 2.5 in (63.5 mm), according to the TEMA standard. BWG thickness is expressed in standard tubes. An increase in BWG value indicates a decrease in tube thickness.

Table 4: Common Tube Layout

Tube OD, in	Pitch type	Tube pitch, in
$\frac{3}{4}$	Square	1
1		$1 \frac{1}{4}$
$\frac{3}{4}$	Triangular	$\frac{15}{16}$
$\frac{3}{4}$		1

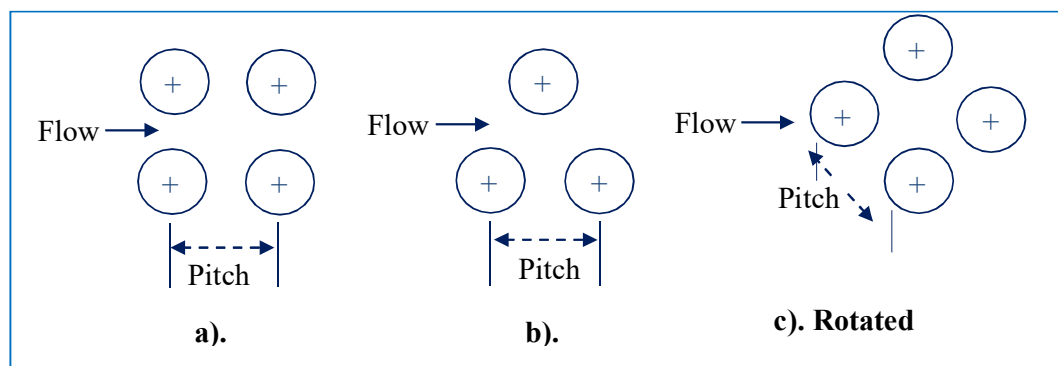


Figure 9: Heat Exchanger Tube Layout

Tube sheet

The tube or tube bundle is supported by tube sheets. In the case of a U-tube heat exchanger, only one tube sheet is required to hold the tube. In a fixed tube heat exchanger, two tube sheets are used.

Baffles

Baffles are used to create turbulence on shell side fluid for proper heat transfer. Also baffles support the tube bundle. Basically 25% baffle cut are used in shell and tube heat exchanger.

Selection of Fluids for Tube and The Shell Side

Table 5: Guidelines for Placing the Fluid in Order of Priority

<i>Tube-side fluid</i>	<i>Shell-side fluid</i>
Corrosive fluid	Condensing vapor (unless corrosive)
Cooling water	Fluid with large temperature difference ($>40^{\circ}\text{C}$)
Fouling fluid	
Less viscous fluid	
High-pressure steam	
Hotter fluid	

2.9 Design of centrifugal pump

A device used to transfer a fluid from one place to another place. It worked on the principle of conservation of energy. Its capacity decides based on how much fluid have to transfer with in a time.

2.9.1 Flowrate

How much the volume has to be pumped by a pump per unit of time is denoted by Q and has unit of m^3/h , l/s , etc. based on pipe diameter pump flowrate is decide. Figure 10 Selection of Pump Based on Head shows that

Under 10 m	From 10 to 100 m	From 100 to 1,000 m	From 1,000 to 10,000 m	From 10,000 m and over
One-stage centrifugal pumps				
		Multistage centrifugal pumps		
Axial flow pumps (head is up to 20-30 m)				
	Piston pumps			
	Screw pumps			
			Plunger pumps	
Vortex pumps				

Figure 10: Selection of Pump Based on Head

2.9.2 Head

The unit of pumped medium mass is attributed to the energy imparted by the pump. The letter H denotes a unit is in meters. Head is nothing but how much water pump will lift.

Under 10 m ³ /h	From 10 to 100 m ³ /h	From 100 to 1,000 m ³ /h	From 1,000 to 10,000 m ³ /h	From 10,000 m ³ /h and over
One-stage centrifugal pumps				
		Multistage centrifugal pumps		
		Axial flow pumps		
Piston pumps				
Screw pumps				
Plunger pumps				
	Vortex pumps			

Figure11: Selection of Pump Based On Flowrate

2.9.3 Power

Amount of energy required to operate pump, which is the amount of energy directly used to move the pumped medium. Leakages and bearing friction can cause some power to be lost.

These quantities are determined by the performance factor. The calculation of these characteristics may vary depending on the type of pump.

3. REACTION KINETICS

The assumption of batch operation

1. The contents of the tank are well mixed
2. The reaction does not occur to an appreciable degree until filling & start-up procedures are complete

3.1 Procedure to Determine the Reaction Kinetics

1. Setup a batch with feasible formulation as per literature.

Table 6: Batch formulation

Component	Molecular Weight (g/mol)	Weight (g)	Moles (mol)	OH/COOH Ratio
Adipic Acid	146.14	120	0.82	1.52
Neopentyl Glycol	104.15	130	1.25	
Batch Size		250		

2. Start the reactor and set the temperature to 150°C. Increase the temperature the temperature by 10°C after every 1 hour.
3. Note time (in min) and draw a sample from the batch reactor every 10 minutes; after the reaction temperature reaches 150°C. Apply vacuum and increase it to 30 mmHg (of vacuum) over a period of 2 hours.
4. Weigh the sample (in g)
5. Add solvent (Acetone-10 ml) and indicator (Phenolphthalein-2 drops) to the sample flask.
6. Titrate it against Alcoholic KOH and note down the burette reading (**B.R.**)
7. Calculate Acid Value (in mg KOH/g); **A.V.**

$$\text{Acid value} = \frac{5.61 \times \text{B.R.}}{\text{wt. of sample}} \quad (2)$$

8. Calculate concentration (in mol/l); **C_A**

$$C_A = \frac{\text{A.V.} \times \text{Density of product}}{56.1} \quad (3)$$

9. Plot a graph concentration vs time
10. Find slope at every point.
11. Calculate Rate of Reaction (mol/l min); **-r_A**

12. Calculate $\log(C_A)$
13. Calculate $\log(-r_A)$
14. Plot $\log(C_A)$ vs $\log(-r_A)$
15. Calculate slope and determine order of reaction; n
16. Note y-intercept and calculate rate constant; k

4. CONCLUSION

The study was made on the kinetics of esterification reaction of adipic acid and neopentyl glycol. The kinetic study involved the use of differential and integral method of analysis. It was found that the esterification reaction between adipic acid and neopentyl glycol is a second order reaction.

Further, with a basis of 10 tons, a theoretical plant design was performed. Batch reactor based on the reaction kinetics was design. By-product, i.e. water along with nitrogen is removed from the top of the reactor which is condensed in a condenser. Thus, a condenser was also designed for condensing condensable as well as non-condensable fluids. Further an agitator was designed in detail for the homogenous mixing of the reactants. Selection of impeller and power calculations for the agitator was performed. To maintain temperature in the batch reactor, a coil was welded to the vessel wall that would act as the jacket through which Dowtherm fluid at high temperature is pumped thus heating the reactor.

Further pumps for pumping the Dowtherm fluid were also designed. Frictional losses during pumping were considered using Moody's chart. Same was applied to the pump that is used to pump cooling water to the condenser.

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