



**ADDIS ABABA INSTITUTE OF TECHNOLOGY  
SCHOOL OF MECHANICAL AND INDUSTRIAL ENGINEERING  
THERMAL ENGINEERING STREAM**

**DESIGN OF BIODIESEL REACTOR HEATED  
BY STEAM FROM JATROPHA CAKE BOILER**

By

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A paper submitted to the School of graduate studies of Addis Ababa University in partial fulfillment for the requirement of Masters of Science in Mechanical Engineering (Thermal Engineering)

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June, 2019 G.C.

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## Signature Page

Addis Ababa University

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This is to certify that the thesis prepared by Bilisumma Yadessa Abalti entitled: **Design of Biodiesel reactor heated by steam from Jatropha cake boiler** and submitted in fulfillment for the requirement of Masters of Science in Mechanical Engineering (Thermal Engineering) complies with the regulation of the university and meets the accepted standards with respect to originality and quality.

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## DECLARATION

I hereby certify that the work which is being presented in this Thesis entitled, ” *Design of biodiesel reactor heated by steam from jatropha cake boiler* ” in partial fulfillment of requirement for the award of the degree of Master of Science in Mechanical Engineering with specialization in Thermal Engineering submitted to school of Mechanical and Industrial Engineering of Addis Ababa University ,it is authentic record of my own work carried out under the supervision of Dr.Ing.Demis Alemu and Mr Sine Girma (PhD candidate). The work refers other researcher’s works that is duly listed in the references section.

The matter presented in this thesis has not been submitted for the award of any other degree of this or any other university.

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## ABSTRACT

Since in the last century, fossil fuel resources are being depleted at alarming rate due to rapid industrialization. Combustion of large quantity of fuel resulted in emission of pollutant and Carbon dioxide and caused greenhouse effect that caused global warming. The remedy of global warming is to substitute fossil fuels by renewable energy. Among the renewable energy sources, biodiesel is a fuel that can substitute diesel fuel. Biodiesel is produced by transesterification of plant oils. Jatropha is one source of biodiesel which is non-edible by human being and animals. Instead of using edible vegetable oils, use of jatropha oil does not endanger food security.

The generation of biodiesels needs reactors in which the chemical reaction or transesterification takes place. When biodiesel is produced from jatropha seed during oil extraction, jatropha cake is obtained as byproduct. The main objective of this thesis is to design appropriate reactor for Biodiesel which is heated by steam from jatropha cake boiler so that the process will be self-sufficient in thermal energy use. The design of jacketed reactor is done by analytical and computational methods through Ansys fluent release 17.2 to assure proper mixing and uniform reaction temperature is achieved. The steam jacket around the reactor is insulated to reduce heat losses.

The jacketed reactor is designed for steam annular area as heat exchanger without fluid contact. The temperature of the jatropha oil is raised from 30 to 80 degree Celsius by transferring of heat energy from steam boiler which is the maximum temperature. This heat is required to reduce the retention time of jatropha oil during reaction with ethanol oil to produce biodiesel. No heat loss is happened at the conical shape of the reactor and heat is transferred from the wall of the reactor to the batch fluid to raise the temperature of the batch fluid from 303 to 353K for 500s heating process by using 412.16kJ capacity of jatropha cake boiler which is used 75 kg of jatropha cake. From this capacity of boiler, 269.81kJ heat energy is transferred by convection and conduction heat transfer system to heat 75kg of batch reactant in the reactor. The heating time of jatropha oil through convection heat transfer through reactor is 500s.

**Key words:** Biodiesel, Jatropha, Batch reactor, Jacketed Heat transfer

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## **DEDICATION**

I devote this work for my lovely mother, Wili Tolassa Mulata who passed away while I am on study of high school for her bearing me and grow me up well from the beginning of pregnant to till my high school study. She was a mentor, visionary and exemplary to me although she did not go to formal education. I benefited a lot from her wisdom and affection as a child and adult man until she left me without a mother. She is so special and kind to me in shaping my destination. May her soul rest in peace in the hands of the heavenly father!

## Table of Contents

DECLARATION.....	I
ABSTRACT .....	I
ACKNOWLEDGMENTS .....	II
DEDICATION.....	III
Table of Contents.....	IV
LIST OF FIGURES .....	VII
LIST OF TABLES.....	VII
CHAPTER ONE.....	1
BACKGROUND AND JUSTIFICATION.....	1
1.1. Background.....	1
1.2. Objectives .....	2
1.4. Thesis organization .....	2
1.5. Problem of statement .....	2
1.6. Expected outcome.....	4
CHAPTER TWO.....	5
LITERATURE REVIEW .....	5
2.1. History of biodiesel use .....	5
2.2. Physical and chemical properties of biodiesel and diesel.....	5
2.3 Specifications of biodiesel .....	6
2.4 Biodiesel production by transesterification .....	7
2.4.1. Kinetics of alkaline-catalyzed transesterification reactions.....	9
2.4.2. Transesterification reaction process.....	9
2.4.3. Variables affecting the yield of transesterification reaction .....	11
2.5. Environmental advantages .....	12
2.6. Economic feasibility .....	13
2.7. Steam boiler for reactor heating system.....	13
2.7.1. Boiler description .....	14
2.7.2. Fire tube boiler fueled by biomass .....	14
2.7.3. Steam generation from jatropha cake.....	16
2.7.4. Modes of heat transfer in fire tube boiler.....	18
2.8. Jacketed vessel analysis .....	18
2.8.1. Heat transfer in the jacketed reactor using steam from jatropha cake boiler .....	19

2.8.2. Application of Fire Tube Steam boiler for heating of batch reactor .....	19
2.9. Selection of reactor system for Jatropha oil.....	20
2.9.1. Jacketed vessel or jacketed batch reactor .....	20
2.9.2. Factors influencing agitation .....	21
CHAPTER THREE .....	25
MATERIALS AND METHODOLOGY.....	25
3.1. Materials .....	25
3.1.2. Material selection .....	25
3.1.3. Material selection for simple jacket .....	26
3.2. Methodology .....	27
3.2.1. Selection of stirred batch reactor.....	27
CHAPTER FOUR .....	30
DESIGN ANALYZING OF REACTOR HEATED BY STEAM BOILER.....	30
4.1. Sizing of batch reactors.....	30
4.2. Calculation of reactor unit .....	30
4.3. Designing condition for reactor vessel .....	31
4.3.1. Determination of temperature for biodiesel formation .....	33
4.3.2. Impeller calculation.....	34
4.3.3. Power calculation .....	35
4.3.4. Analyzing the amount of steam generated from jatropha boiler .....	37
CHAPTER FIVE .....	40
MODELING OF HEAT TRANSFER IN JACKETED BATCH REACTOR .....	40
5.1. Batch heating and cooling of fluids .....	42
5.2. Methods of Heat transfer in jacketed batch reactor .....	43
5.2.1. Direct heat transfer process .....	44
5.2.2. Indirect heat transfer .....	45
5.2.3. Heat transfer from hot side fluid-partition.....	45
5.2.4. Thermal Conduction in the Partition .....	46
5.3. Heat transfer analysis of agitated vessel .....	46
5.3.1. Heat transfer correlations for agitated fluids.....	46
5.4. Heat transfer in agitated reactor .....	47
5.4.1. Design equation of heat transfer .....	47
5.5. Energy balance in jacketed reactor .....	52

5.6. Computational modeling of jacketed reactor .....	54
5.6.1. Geometry and mesh generation .....	54
5.6.2. Model and Assumptions .....	55
5.6.3. Control Equations .....	56
CHAPTER SIX 6.....	58
RESULTS AND DISCUSSION.....	58
6.1. Numerical simulation.....	58
6.1.1. Simulation result of stirred reactor system.....	61
6.2.1. Jacketed vessel simulation result.....	63
CHAPTER 7 .....	70
CONCLUSION AND RECOMMENDATION .....	70
REFERENCE .....	72
APPENDIX .....	78

## LIST OF FIGURES

Figure 2. 1: Transesterification reaction .....	8
Figure2.2: The stoichiometry of the transesterification of triglyceride .....	9
Figure 4.1: over all dimensions of Batch reactors with jacketed heat exchanger .....	33
Figure 4.2: (a) represents 3D of assembled jacketed agitated reactor, (b) over all dimensions of jacketed agitated reactor .....	37
Figure 5.1: Assembled jacketed vessel with two inlets and one outlet .....	42
Figure 5.2: Temperature curve at the partition.....	45
Figure 5.3: Resistance diagram for heat transfer from the jacket to the process.....	48
Figure 5.4: Stirred jacketed vessel assembly.....	55
Figure 5.5 overall part names of the reactor with 3D drawing of jacketed reactor .....	55
Figure 6.1 (a) represents jacketed agitator vessel (b) jacketed vessel section view of the model.....	59
Figure 6.2 Meshing of the assembled vessel system discretized at different elements.....	60
Figure 6.3 velocity vector of the incoming batch fuel in the chemical reactor .....	61
Figure 6.4 (a) and (b) shows the plane section of turbulence kinetic energy contour and pressure contour in stirred reactor during chemical reaction respectively. ....	62
Figure 6.5 the stirring or mixing of fuel system with the ethanol with baffled reactor.....	62
Figure 6.6. Solution iteration of transient fluid flow convergence diagram.....	63
Figure 6.7 from a-n shows temperature distribution during heating of batch reactor at different times .....	67
Figure 6.8 stream line flow of incoming fuel in the batch reactor .....	68

## LIST OF TABLES

Table 2.1. Physical and chemical properties of vegetable oil sources and petroleum diesel[10].....	6
Table 2.2: General parameters of the quality of biodiesel [1].....	7
Table 2.3. Different types of fire tube and consumption fuels .....	14
Table 2. 4. proximate and calorific value of biomass samples[42]. .....	17
Table 2. 5. Fuel properties of mineral diesel, Jatropha biodiesel, Jatropha oil .....	23
Table 3.1. Physical properties of metals[58] .....	25
Table 3.2: Chem. Eng.et al.,[59] has given the following rules for selecting the jacket type. ....	28
Table 4.1: Standard Stirred Tank Reactors source Ref.[60].....	30
Table 5.1: Exponent for different impellers and Re regimes .....	41

# CHAPTER ONE

## BACKGROUND AND JUSTIFICATION

### 1.1. Background

Nowadays energy demand is on increase in alarming rates caused by industrialization and increasing of population in the world. The world is switching to renewable energy sources to mitigate the depletion of fossil fuel and the global warming. In addition to these problems, the demand for energy is on increase without increasing energy supply. The solution for transport sector and other sectors to alleviate the problem is to use biofuels instead of using petroleum derivative fuels at least partially. Vegetable oils, tallows, and kitchen oil recovery can be used to generate biodiesel through different mechanical and chemical systems. Among them vegetable oils, this work uses none-edible jatropha oil due to its non-competitiveness with food security[1]. Jatropha curcas plant will yield biodiesel fuel after different process including the preparation of the plantation. This study focuses on the production of biodiesel from jatropha curcas oil by using appropriate reactor design. The reactor design involves use of heat transfer from steam jacketed vessel. Therefore, the design of reactor is done through the consideration of heat generated by steam from boiler that uses Jatropha seed cake as a fuel. In the reactor, the main chemical reaction that converts Jatropha oil to biodiesel occurs. The design of this reactor will consider the chemical property of the reactants to select appropriate material. Worldwide, methanol alcohol is used for the production of biodiesel from jatropha oil. Since ethanol is produced from sugar plants in Ethiopia and methanol is toxic. Ethanol is considered the best path way for the sustainable production of biofuel by transesterification method (ethanolysis) than that employed by methanol (methanolysis) for small scale production in Ethiopia. Methanolysis is a multiphase reaction, which occurs only at the boundaries of methanol droplets dispersed in the vegetable oil phase, ethanolysis, on the other hand, can be approximated by a single-phase reaction while in stirred tank reactors. Modeling and simulation of multiphase reaction like methanolysis usually requires prohibitive computational resources, while ethanolysis requires only a commercial CFD code in which equations for the reaction kinetics can be introduced as source terms in the mass conservation equations implemented in the software.

Thus, the aim of this work was to perform a CFD simulation heat transfer during transesterification of ethanolysis in a baffled stirred reactor, with reaction rates being evaluated by solving a set of differential equations describing as source terms in mass conservation equations.

Excess ethanol is used to facilitate the reaction and sodium hydroxide catalyst is selected for the transesterification process. The chemical reaction of jatropha oil is completed if the molar ratio of ethanol to oil, reaction rate, catalyst, and temperature parameters are correctly used. If one of this parameter is missed, the formation of soap and glycerol is produced. The reactor selected is jacketed batch reactor.

## **1.2. Objectives**

The general objective of this thesis is to design appropriate reactor for Biodiesel which is heated by steam from jatropha cake boiler so that the Biodiesel production process will be self-sufficient in use of thermal energy

## **1.3. Specific objectives**

The specific objectives are:

- Design of jacketed reactor for the production of biodiesel
- Design of appropriate agitator for facilitating of heat transfer in the reactor and mixing of the reactants to increase its turbulence
- Modeling of the batch reactor heated by steam to determine heating time
- Reduction of retention time during the production of biodiesel by transferring steam energy through jacketed wall to the batch reactor

## **1.4. Thesis organization**

This thesis is divided into sub-sections. The first part is literature review on the work which was done related to this study. The second deals with the materials and methodology used for the work. The next part deals with the result and discussion. The final part is concerned with conclusion and recommendation of the work.

## **1.5. Problem of statement**

In our country Ethiopia, energy generation relies on non-renewable fossil fuels which are mostly imported from abroad. Now days the transformation of the economy is taking place

from agricultural system to industrialization and also the policy of the country focus on industrialization as a way out of poverty. Therefore the demand for diesel fuel is on increase within these non-renewable and limited sources [2]. Of the total amount of energy imported nearly 50% is consumed by the transport sector [3]. If the demand and supply of this energy miss-match, it will have an impact on economic sustainability and development of the country [4]. Besides economic growth problem, this source of energy cause environmental problem such as greenhouse gas emission and acid rains [5]. To mitigate the above problems, developing of alternative energy source is recommendable. Generally the problem of fuel in transportation sector can be solved by generating of biodiesel from *Jatropha curcas* plant which yields oil by using continuous chemical reactor. But, for small scale production of biodiesel in rural area for agricultural use to produce fuel as for grain mill engine, small generator, pump engine and small tractors, geometrical simple and energy self-sufficient reactor can be used. Hence, the batch reactor shall have a steam jacket or annular space where the steam from *jatropha* cake boiler condenses transferring heat. This is to recover energy from waste products instead of using electric and coal to generate energy in steam boiler. Investment and running cost to produce the biodiesel by heating steam boiler (using *Jatropha* cake as fuel) would be cheaper than heating by electric energy. This system saves energy loss and recovering of waste product of *jatropha* seed and kernels. Fuel cost expense will be reduced and conservation of energy will be achieved. Therefore, this work concentrates on designing a batch reactor which was heated by *jatropha* cake steam boiler.

## **1.6. Expected outcome**

Biodiesel reactor design using steam from jatropha cake as fuel is the major outcome of this work. The cost of coal and electric energy is reduced since jatropha cake is used as a source of fuel for steam boiler. The environmental pollution will be reduced by decreasing the amount of sulphur in the fuel. As result, the cost of production of biodiesel will be reduced.

The operation of the reactor is simple and the feeding of the fuel is batch process and the complexity of flow rate is avoided.

## CHAPTER TWO

### LITERATURE REVIEW

#### 2.1. History of biodiesel use

Biodiesel is a renewable, biodegradable and environmentally friendly source of fuel used as diesel engine. Biodiesel is produced from vegetable oil, animal fat and or from waste cooking oil. It is comprised from fatty acid alkyl ester (FAAE). Biodiesel can be used purely as diesel engine or blending with diesel fuel. The similarity of biodiesel fuel and diesel fuel shows that biodiesel is an alternative source of fossil fuel [6]. Due to frequent use of petrol fuel in transport sector, agricultural sector and power generating engines , high emission of carbon dioxide (CO<sub>2</sub>) ,carbon monoxide (CO), sulphur dioxide (SO<sub>2</sub>) and nitrogen oxides (NO<sub>x</sub>) released to the environment. These pollutants are the result of incomplete combustion of petrol fuel. This problem needs alternative system of renewable fuel from vegetable oil and animal fats. This fuel is known as biodiesel as it is derived from biological resources. Biodiesel has less of sulphur, water and carbon, more content of oxygen when compared with convention diesel fuel. Therefore ,biodiesel has less amount of SO<sub>2</sub>,CO<sub>2</sub> and NO<sub>x</sub> during combustion in diesel engine which is environmental friendly[7]. A lot of researchers worked on the conversion of biodiesel from jatropha curcas seed and shells [8,9].

#### 2.2. Physical and chemical properties of biodiesel and diesel

The physical and chemical properties of biodiesel and diesel are listed in table 2.1. The volumetric heating value is the heat released when the known quantity of fuel is burned under specific conditions. The Cetane number expresses the ignition quality of the fuel and the flash point expresses the tendency of the fuel to form flammable mixture with the air. The high Cetane number of biodiesel improves ignition delay of air-fuel mixture during engine running which can reduce engine noise. The high flash point of biodiesel fuel is safe for transportation and storage of the fuel than the petrol fuel. The viscosity of biodiesel is slightly higher than petrol fuel but in acceptable variation from American Society for Testing and Material (ASTM) standard. And also at low temperature, the cloud point and freezing point of the biodiesel is low compared to petrol.

Table 2.1. Physical and chemical properties of vegetable oil sources and petroleum diesel[10].

Vegetable oil methyl ester	Kinematic viscosity (mm <sup>2</sup> /sec)	Cetane number	Volumetric heating value (MJ/L)	Cloud point(°C)	Flash point (°C)	Density (gm/cm <sup>3</sup> )
Rape seed	4.2 (40°C)	51-59.7	32.8	-----	-----	0.882(15 °C)
Peanut	4.9 (37.8 °C)	54	33.6	5	176	0.883
Soybean	4.5 (37.8 °C)	45	33.5	1	178	0.885
Babassu	3.6 (37.8 °C)	63	31.8	4	127	0.879
Palm	5.7 (7.8 °C)	62	33.5	13	164	0.880
Sun flower	4.6 (37.8 °C)	49	33.5	1	18.3	0.860
Tallow	-----	-----	-----	12	96	-----
Used rape seed	9.48 ( 30 °C)	5.3	36.7	-----	192	0.895
Used common oil	6.23 ( 30 °C)	63.9	42.3	-----	166	0.884
Diesel fuel	1.2-3.5(40 °C )	51	35.5	----	-----	0.83-0.84

The chemical composition of fatty acid alkyl ester (FAAE or biodiesel) shows 77% CO reduction, 10-12% of O<sub>2</sub> and the same of content within petrol fuel. Biodiesel has negligible amount of sulphur and phosphorous with non-aromatic contents. This result shows biodiesel is environmental friendly compared to fossil fuel due to less emission of CO, hydrocarbon compounds and aromatic fuel. Therefore biodiesel is a candidate for fuel in diesel in the world due to its environmental friendly[11] .

### 2.3 Specifications of biodiesel

To guide the fuel problem and limit the fuel hazards and to promote engine life, different standards were created in different country. The first standard was developed in Austria since 1991 on rapeseed oil of methyl ester, followed eventually by North America (ASTM D6751) and European standards (EN 14214) [12]. The Canadian General standard board (CGSB) recognizes (ASTM D6751) as Canadian biodiesel standard. The density and Cetane number of biodiesel is depending on the type of vegetable oil. Impurities found in the vegetable oil such as free and total glycerol ( total glycerol is free glycerol and glycerol

bound as mono-,di-,and triglycerides) ,water ( moisture) ,free fatty acid ( by limiting the number of acid ) and residual alcohol ( by limiting the flash point ) ,need to be limited in biodiesel because their presence can lead to fuel degradation during storage and to significant operational problem in the engine deposits. The viscosity also represents unreacted triglycerides.

Table 2.2: General parameters of the quality of biodiesel [1]

Parameters	Austria (ON)	Czech republic (CSN)	France (Journal official )	Germany (DIN)	Europe (EN 14214)	North America (ASTM D6751)
Density at 15 °C( gm/cm <sup>3</sup> )	0.85-0.89	0.87-0.89	0.87-0.89	0.876-0.89	0.86-0.9	-
Viscosity at 40 °C (cst)	3.5-5	3.5-5.0	3.5-5.0	3.5-5.0	3.5-5.0	1.9-6.0
Flash point ( °C)	100	1110	100	110	>110	130
CFPP**(°C)	0/-5	-5	-	-10/-20	-	-
Pour point (°C)	-	-	--10	-	0/-0.5	-
Cetane number	≥49	≥48	≥49	≥49	≥49	≥51
Acid number (mg KOH/g)	≤0.8	≤0.5	≤0.5	≤0.5	≤0.5	≤0.5
Carbon residue (%)	0.05	0.05	-	0.05	<0.03	0.05
Methanol /Ethanol (% mass)	≤0.2	-	≤0.1	≤0.3	≤0.2	-
Ester (contents) (% mass)	-	-	≥96.5	-	≥96.5	-
Mono-glyceride (% mass)	--	-	≤0.8	≤0.8	<0.8	-
Di-glyceride (% mass)	-	-	≤0.2	≤0.4	<0.2	-
Triglyceride (% mass )	-	-	≤0.2	≤0.4	<0.4	-
Free glycerol( % mass)		≤0.02'	≤0.02	≤0.02	≤0.02	≤0.02
Total glycerol (% mass)	≤0.24	≤24	≤0.25	≤0.25	≤0.25	≤0.24
Iodine number	≤120	-	≤115	≤115	120	-

CFPP\* --- cold-filter plugging point.

#### 2.4 Biodiesel production by transesterification

There are four primary methods of using vegetable oil as biodiesel fuel: Direct use and blending, emulsification, transesterification and pyrolysis (thermal cracking) method. The

most appropriate to use for biodiesel production method is transesterification, which the reaction is takes place with alcohol to form ester and glycerol.

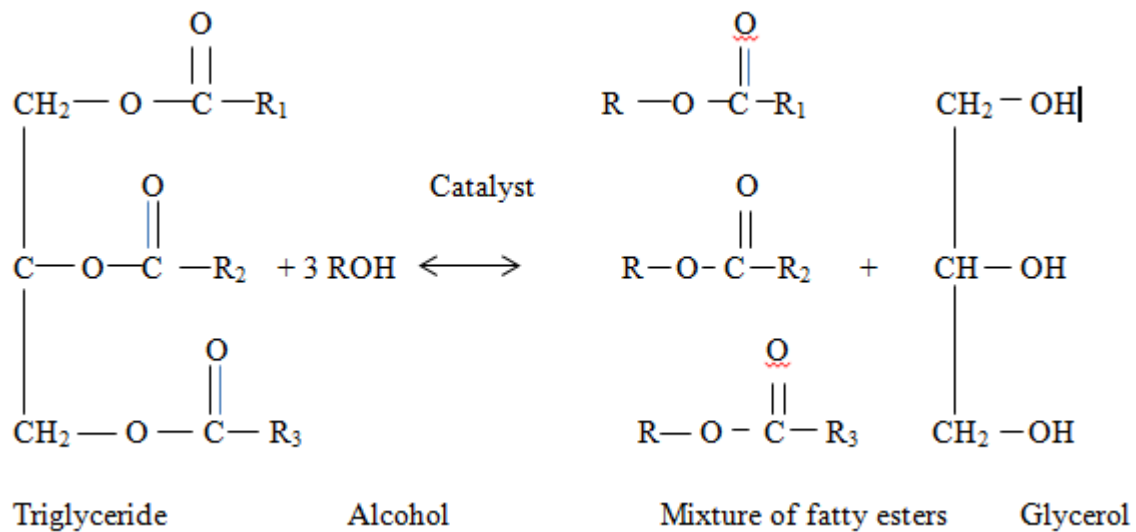


Figure2. 1: Transesterification reaction

R<sub>1</sub>, R<sub>2</sub>, and R<sub>3</sub> are hydrocarbons chains called fatty acids. For common vegetable oils and animal fats, they are usually fatty acids of 16-18 carbons with 0-3 double bonds, which are mostly stearic, palmitic, oleic, linoleic, and Linolenic. These types are:

Palmitic: R- (CH<sub>2</sub>)<sub>14</sub> - CH<sub>3</sub>, 16 carbons, with no double bonds (16:0)

Stearic: R- (CH<sub>2</sub>)<sub>16</sub> - CH<sub>3</sub>, 18 carbons, 0 double bonds (18:0)

Oleic: R - (CH<sub>2</sub>)<sub>7</sub>=CH (CH<sub>2</sub>)<sub>8</sub> CH<sub>3</sub>, 18 carbons, 1 double bond (18:1)

Linoleic: R- (CH<sub>2</sub>)<sub>7</sub> CH =CH-CH<sub>2</sub>-CH=CH (CH<sub>2</sub>)<sub>4</sub>CH<sub>3</sub>, 18 carbons, 2-double bonds (18:2)

Linolenic: R- (CH<sub>2</sub>)<sub>7</sub>CH=CH-CH<sub>2</sub>-CH=CH-CH<sub>2</sub>-CH=CH-CH<sub>2</sub>-CH<sub>3</sub>, 18 carbons, 3 double bonds (18:3). Different alcohols can be used in transesterification such as methanol, ethanol, propanol and butanol. Methanol and ethanol is used most frequently, especially methanol is used due to its low cost and easily recovery. To force the chemical reaction to the right, excess alcohol stoichiometry (3:1) is needed. It is common to use molar ratio ranging from 6:1-12:1 to yield high ester. Alkaline -catalyst is extensively used rather than acid catalyst. Alkaline catalyst reaction is 4000 times faster than the same amount of acid Catalyst. Acid catalyst can cause corrosion on the industrial equipment during transesterification. Therefore

Alkaline-catalyst is used in industrial equipment due to its less- corrosive activity. Sodium Alkoxides is the most efficient and commonly used alkaline catalyst [28, 29].

#### 2.4.1. Kinetics of alkaline-catalyzed transesterification reactions

The transesterification reaction is represented by a number of consecutive reversible reactions as indicated in figure 2.2 below. The first step is conversion of triglycerides to di-glyceride, which is followed by conversion to mono-glyceride. Mono-glyceride is converted into methyl ester (ethyl ester) and glycerol. The stoichiometry of transesterification reaction is as shown below.

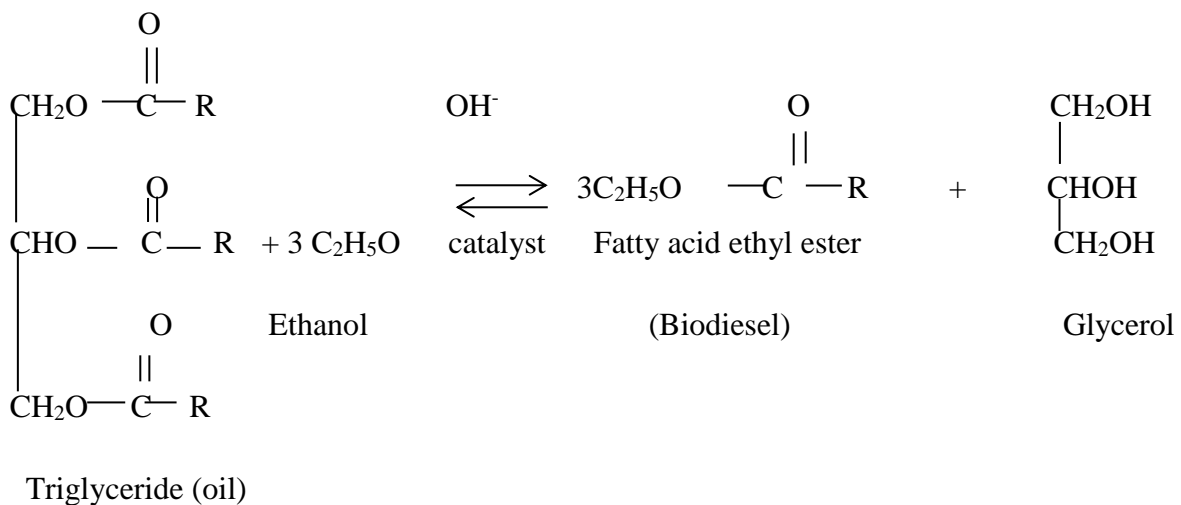


Figure 2.2: The stoichiometry of the transesterification of triglyceride

#### 2.4.2. Transesterification reaction process

Transesterification reaction is the major process of biodiesel production among other methods. To precede the transesterification reaction, the following procedures are taking place.

##### 1. Oil heating

To speed up the reaction and to removes water, jatropha oil is boiled at 105-112<sup>0</sup>C for at least 30 minute[15,31]. Heating is stopped after the water bubble is no there in the oil. When water is present, particularly at high temperature, it can hydrolyze the triglyceride into diglyceride and free fatty acid. Stirring is used for reducing the exposition of oil from more temperature. After all water residues are removed from the oil it should be cooled too little temperature which is lower than the boiling temperature of ethanol alcohol.

## 2. Mixing of Sodium hydroxide catalyst (NaOH) and Ethanol alcohol

Mixing of NaOH catalyst and ethanol is to form ethoxide from the two substances. Ethanol is selected due to the following reasons: due to its abundance location in the market and it is a renewable sources of energy from molasses of sugar industry and farming areas.

## 3. Transesterification reaction

In transesterification reaction, reactants initially form two phases of liquid system. The reaction is controlled by diffusion and at low temperature diffusion process is low. In order to speed up the reaction of Ethoxide and oil, the reaction mechanism is required. Experimental result of Gerhard Knothe [17] shows that reaction is affected by mixing intensity. Best reaction takes place at mixing speed greater than 200rpm. This mixing is significant only for low speed reaction. For single phase, mixing speed is insignificant and the rate is influenced by reaction temperature [33,34] . Optimum temperature is required for yielding of efficient biodiesel under single phase reaction.

## 4. Draining of glycerol

Pure biodiesel is produced after draining of glycerol as byproduct. Due to weight difference glycerol settle to bottom and the color of the products are different. Glycerol is dark while biodiesel is yellow color. For the settlement of glycerol, it takes maximum 12 minute. The viscosity of glycerol is high compared to biodiesel. The reduction of viscosity from biodiesel is necessary by removing glycerol byproduct from the fuel.

## 5. Biodiesel washing

Purification of biodiesel takes place under different method. Among them, distillation method is simple and less costly to be under taken. Washing of the fuel by water wash only and air bubble wash. The combinations of the two methods are used in most case. Hot water prevents the precipitation of saturated fatty acid ester and retarding of emulsion formation during water washing. Warm water above 40-60°C [20] is misted (condensed water vapor) above the fuel. The amount of water needed for washing is 25%-100% volume of washed oil [36,37] and can be drained off throughout the washing process. After water washing is draining off, air bubble used for washing of biodiesel. Air bubble is agitated roughly to clean the fuel. During the washing process, gentle agitation is required to avoid emulsion.

## 6. Biodiesel drying

After washing of biodiesel, the drying of the fuel into clear crystal is needed. This can be done by putting in open sun for a few day or heating to around 49<sup>0</sup>C. Another common method is recirculating of the biodiesel from the bottom drying tank trough the spraying or shower suspended above the top of above tank. This will increase contact with air and reducing the humidity of the biodiesel [37].

### 2.4.3. Variables affecting the yield of transesterification reaction

There are different variables which can affect transesterification reaction. The following are the variables:

#### a. Effect of ethanol to oil mass ratio

The molar ratio of ethanol and crude jatropha oil is the main work for the conversion to biodiesel. Excess ethanol is used for the conversion of crude jatropha oil into biodiesel by preventing soap formation. High ethanol /oil mass ratio increases the polarity of the reactant mixture, driving the reaction for completion: on the other hand, excess ethanol dilutes the catalyst concentration, leading to reduction in oil conversion. The analysis result showed that the ethanol/oil molar ratio increases reduces the actual yield of the biodiesel. The biodiesel yield increases till the threshold limit of ethanol/oil molar ratio concentration[23].

#### b. Effect of temperature

The rate of reaction is strongly affected by the reaction temperature. How ever, given enough time, the reaction will proceed to near completion even at room temperature. The maximum yield of esters occurs at temperatures ranging from 60 to 80<sup>0</sup>C. Generally, the reaction should be conducted close to the boiling point of used alcohol (i.e. ethanol, the temperature shouldn't greater than the boiling point which is 80<sup>0</sup>C) at atmospheric pressure for optimum yield. The methanolysis proceeded to completion in 40 minutes at 60<sup>0</sup>C, yielding a methyl ester content of 98.6% w/w. The effect of temperature slightly affects the conversion of crude jatropha oil into biodiesel. Optimum temperature required for yielding of oil is at room temperature. There are advantages of operating at room temperature:

- 1<sup>st</sup> the convenience and safety implication during transesterification and the subsequent neutralization of the catalyst and

- 2<sup>nd</sup> a low operating temperature can reduce the degree of saponification. JAOCS [24] reported that at 50% or more NaOH catalyst concentration was destroyed before 11-12 minute of reaction due to soap formation, where no saponification at room temperature[25].

#### c. Effect of catalyst concentration

NaOH is used as the catalyst of this reaction. Catalyst concentration affects the concentration of ethyl ester formation during transesterification reaction. Ethyl ester concentration is high at 1% NaOH catalyst concentration by weight of oil. Ethyl ester concentration is decreased as ethanol/oil molar ratio increases. This is happened due to the dilution of catalyst by excess ethanol alcohol.

#### d. Effect of time

The conversion rate is increases with reaction time. Freed B. et al.1984,transesterified peanut, cotton seed, sun flower and soybean oils under the conditions of methanol to oil ration of 6:1, 0.5% sodium methoxide catalyst and 60 °C. An approximate yield of 80% was observed after 1min for soybean and sunflower oils. After 1h, the conversions were almost the same for all four oils (93-98%). Ethyl ester concentration increased as the reaction time increases. This is due to the increase in mixing dispersion of ethanol in oil phase with reaction time[18].

### **2.5. Environmental advantages**

Before one hundred years ago, Rudolf Diesel tested vegetable oil as an alternative fuel source. Between 1930 and 1940, biodiesel was used for emergency case. Research on biodiesel fuel is not developed due to low cost of crude oil. Recent studies was concerned on renewable source of fuel from vegetable oil mainly due to the cost of fossil fuel and emissions such as carbon dioxide which forced researchers to investigate environmental friendly energy sources [26]. In addition to the above advantage, pure biodiesel or blending with petrol is used in a plant and can be domestically developed. In a study performed in Idaho University, biodegradability by microorganisms in water is above 95% in 28 days. During the same time, petrol fuel degradability is only 40% [27]. Compared to petrol fuel, biodiesel combustion emission such as particulates SO<sub>x</sub>, carbon monoxide, unburned hydrocarbon and soot are small. A slight increase in NO<sub>x</sub> can be reduced by delaying ignition timing in engine[28]. A life cycle study carried out shows pure biodiesel (B100) in

urban buses showed a substantial reduction in particulate matter (32%), CO (35%) and SO<sub>x</sub> (8%) relative to petrol fuel.

## **2.6. Economic feasibility**

Despite its advantages socio-economic and environmental benefits, the cost of biodiesel is great obstacle. As Martin B,[29] from economic feasibility of oil seed and animal fats accounts US\$ 0.30 to 0.67/L including meal and carbon credits.

## **2.7. Steam boiler for reactor heating system**

A boiler means a closed vessel in which steam can be generated for use of external application of heat which wholly or partially under pressure when is shut off but does not include a pressure vessel:

- With capacity less than 25L
- Which is less than 1 kilogram per centimeter square design gauge pressure and working gauge pressure [30].

In simple words, boiler is a closed vessel created from stainless steel. Its function is to transfer heat generated by the combustion of fuel to water and ultimately to generate steam. Steam generated is used for industrial applications. Fire tube boiler is consisting of a shell which is filled with water and perforated with tubes, with different configurations of tubes but horizontal tubes arrangement is common. Water is partially filled in the shell and the left space is to accommodate the steam generated during heat transfer from the tube to the water. The horizontal tubes carry flue hot gases of combustion fuel and heat the water inside the shell. The heat generated in the furnace goes out of the tubes heats the water and it goes out from the smoke stack. Fire tube boilers are subdivided into three groups. Namely:

- Horizontal return tubular boiler
- Scotch, scotch marine, or shell boilers have the fire tubes and combustion chamber housed within the shell.
- Fire box boilers have a water jacketed fire box and employ at most three passes of combustion gases

Depending on the construction details, fire tube boilers have tubes configured in one, two, three or four pass arrangements, because the design of fire tube boilers is simple, they are

easy to construct in a shop and can be shipped fully assembled as a package unit. Fire tube boilers have a lower initial cost, are more fuel efficient and are easier to operate.

Advantages of using fire tube boiler are:

- Low cost
- Fluctuations of steam demand can be met easily
- It is compact in size

The good performance of boiler is maximum heat absorption and minimum heat loss.

Table2.3. Different types of fire tube and consumption fuels

Fire tube boiler	Fuel				
	Coal	Fuel oil	Natural gas	Biomass	Refuse –derived
HRT boilers	Yes	Yes	Yes	Yes	Yes
Scotch boilers	Yes	Yes	Yes	No	No
Firebox boilers	Yes	Yes	Yes	Yes	Yes

### 2.7.1. Boiler description

- Many steam boilers are undersized for actual net load.
- Determine the “BTU or J/kg” required for the heat load.
- Add the losses for the pipe lines, transmission or distribution etc.
- correcting for the operating pressure of the boiler
- correct for the feed water temperature of the boiler

Calculated load × pick-up factor (1.5) = gross load BTU/hr

### 2.7.2. Fire tube boiler fueled by biomass

The production of biodiesel from vegetable oil and kitchen wastes uses external heat energy from electrical energy in most time. In Ethiopia, there are alternative fuel source of heat energy which can speed up the chemical reaction of Jatropha oil and ethanol with catalyst to reduce the retention time of the reaction. This can be done by using steam energy generated from biomass fuel burning in the fire tube boiler. Among the biomass, Jatropha cake is the waste product of oil extracted from Jatropha fruit and Jatropha kernel after oil extraction.

After the oil-extraction from the Jatropha seed, 50% of the weights are Jatropha cake. Jatropha cake may contains toxic phorbol esters and disposal of the cake utilization can be used as animal feed (fodder), production as green manure(fertilizer) and as a fuel[31]. The wastes of these products can be occupying large area after a while of biodiesel production. Instead of this it can pollute the environment due to microbial break down at the dump site. Boiler utilizes these waste products as a source of fuel. This calls for an efficient utilization of this biomass as a source of fuel for the industry [32]. If the jatropha cake is properly dried, it can generate energy related to the energy of being generated from petrol fuel[33]. There are two types of solid fuel boiler: fire tube and water tube. The simpler and less expensive boiler type is the fire tube boiler. This type of boiler is generally used for boiler capacities of up to 30 MW and for saturated steam applications less than 30 bar. The fire tube boilers are also simpler to clean and maintain. They are usually employed with a moving grate boiler which has good degree of flexibility in biomass particle size. But water tube boiler is used for higher pressure applications and has a higher efficiency than the fire tube boiler. Boilers are much configured for a particular combustion temperature and air-fuel ratio. Biomass boilers cannot readily switch from, for example wood chip to wood pellets without a shut down and reconfiguration of boiler controls and fuel supply. Where an industrial user requires a constant steam temperature and pressure, care full attention must be paid to the fuel moisture content. If the moisture content is too low for a given boiler design, combustion temperatures will increase and potentially cause problems with both flue gas emissions and ash-melting behavior. There are opportunities to convert fuel fired fire tube boiler by biomass fired boiler. This biomass fueled boiler uses internal furnace for burning of the biomass fuel source and for financial saving. This also eligible for carbon credit [34]. The energy required in the chemical process is by thermal energy in the form of heat from steam and mechanical energy converted from electricity. The design of the boiler is based on the shell and tube determined based on the time it takes the fuel to reach complete combustion. The dropping of steam pressure and temperature indicates the point of complete combustion of the fuel. The properties of steam produced namely: temperature, pressure, enthalpy and other a monitored type of fuel consumed in the fire tube boiler. Based on closed experiment Prentice Hall, [35] determines the formula for the heat generation due to firing of the given fuel.

$$Q = M_s h_g + M_s C_p \Delta T \quad (2.1)$$

$$C_p = 4.2 \times 10^3 \text{ J / kg.k}$$

Where;

Q is heat flow into the feed water kJ/min, Ms is quantity of steam generated, kg/min, and hg is enthalpy of saturated steam at maximum temperature, kJ/kg, Cp is specific heat capacity of water, ΔT is change in temperature. The quantity of steam generated is calculated as:

$$M_s = \frac{Q}{h_g + C_p \Delta T} \quad (2.2)$$

The quantity of heat energy (Q) supplied by the fuel samples was calculated using the product of the calorific energy content of the fuel sample (kJ/kg) and the quantity of the fuel sample per firing time (kg/min). The change in temperature is the difference between the inlet temperature and the final temperature of the feed water in the boiler drum. Also the enthalpy (hg) of the steam in kJ/kg can be obtained from the steam table. The boiler efficiency is based on the ratio of energy in steam generated to the energy supplied by the fuel ( the burning biomass residue per 8 min firing time as stated by Biomass and Bioenergy institute,[36] as follows:

$$\eta_b = M_s \times \frac{(hg - hf)}{q \times C_v} \times 100\% \quad (2.3)$$

Where;

$\eta_b$ = boiler efficiency

$h_f$  =enthalpy of liquid

$q$ =quantity of fuel used in kg/min

$C_v$ =Calorific value of biomass

### 2.7.3. Steam generation from jatropha cake

Biomass is defined as renewable energy sources of carbonaceous wastes from animal and human activities [37]. Nowadays biomass is contributing 14% global energy and 38% developing country energy [38]. Biomass does not add carbon dioxide to the environment as it absorbs the same amount of carbon dioxide during its growth [17,18]. Jatropha wastes such as jatropha cake is used as a source of solid fuel [41]. The combustion of biomass is

different depending on proximate analysis, boiler type, rate of reaction, sizing and segregation of fuel, temperature of the furnace and fuel bed, reducing and oxidizing of atmosphere etc.[42].

Table2. 4. proximate and calorific value of biomass samples[42].

S.No	Feedstock	Moisture%	Volatile matter%	Ash%	Fixed Carbon	Gross calorific value Kcal/kg
1.	Saw dust	13.8	72.9	0.6	12.7	4028
2.	Groundnut shell	10.1	68	2.8	19.1	4008
3	Bamboo leaves	7.7	68.7	12.3	11.3	3756
4	Cotton stack	7.5	70.3	2.5	19.7	3991
5	Prosopis	7.7	78.9	0.5	12.9	4237
6	Coconut husk	13.4	56.7	2.4	27.5	3800
7	Jatropha cake	7.3	65.1	8.3	19.3	4725
8	Rice husk	7.2	61.8	16.4	14.6	3729
9	Sugarcane	4.5	77.1	2.4	16	4547
10	bagasse	11.5	63.4	5.4	19.7	3601
11	Elephant grass	8.2	71.4	4.6	15.8	3789
12	Typha	20.5	63.5	2.1	13.9	3496
13	Castor stack	11.7	66	3.4	18.9	3670
14	Ipomea	17.1	58.7	4.9	19.3	3800
15	Sun hemp	14.8	62.3	6.3	16.6	3434
16	Sesbania	11.3	68.6	3.3	16.8	4090
17	Sesbania seed	13.2	68.7	3.4	14.7	3763
18	Sunhemp seeds	19.2	50.9	11.6	18.3	2945
19	Bringle residue	19.4	54.1	11.2	15.3	2694
20	Tomato residue	21.4	51	7.5	20.4	3105
21	Capsicum	21.7	48.4	13.3	16.6	2335
25	Perry grass	13.4	50.4	19.3	16.9	2126
26	Okhara residue	7.6	71.5	7	13.9	4666
27	Eucheuma	11.3	64.7	1.7	22.3	4273

S.No	Feedstock	Moisture%	Volatile matter%	Ash%	Fixed carbon	Gross calorific value Kcal/kg
28	Seaweed	5.9	32.4	57.9	3.8	1214
29	Spirullina	3.9	47.4	45.8	2.9	1495
30	Powder	6.6	72.7	4.4	16.3	4244
31	Date palm seed	12.5	67.6	2	17.9	4074
32	Algae powder	6.6	72.8	3.4	17.2	4071

#### 2.7.4. Modes of heat transfer in fire tube boiler

For boiler design, the importance of heat transfer is essential. In the convectional three pass and four pass fire tube boilers, small fire portion of heat transfer is in furnace as much as 90% of heat is transferred by the surfaces of fire tubes. Radiation in the fire tube is non-existent when compared to convection heat transfer in the surface of the tubes. In the industrial sized steam boiler as much as twice more area is in the tubes than in the rest of the boiler volume. Furthermore convection heat transfer in furnace is more than radiation heat transfer. The number of boiler tubes is limited by the capacity of the burner to overcome the internal pressure loss. Due to this reason; the general direction in designing fire tube boilers is given to install only as many tubes as necessary.

There are three modes of heat transfer which takes place during energy flows from one section to another section in the form of heat. These are:

- Conduction
- Convection
- Radiation

#### 2.8. Jacketed vessel analysis

To heat or cool pressure vessels, external “jackets” or internal coil is installed. “Jackets” are common in alcohol, food, beverage and chemistry industries. There are different kinds of “jackets”. Simple jackets, spiral jackets, half-pipe coil and dimpled jackets. These heating or cooling “jackets” are the most popular to use because of the following reasons [50].

- It is easy to clean and maintain by applying “clean media”
- All types of fluid can be used for the cooling or heating of the internal contents of the vessel. To heat steam is perfectly applied and to cool glycol or cold water are ideal

- It is easiest way to control velocity, circulation and temperature of cooling or heating contents
- These types of jacket can be constructed from simple materials when compared to vessels.

### **2.8.1. Heat transfer in the jacketed reactor using steam from jatropha cake boiler**

Endothermic energy is needed to speed up the chemical reaction of jatropha oil with ethanol at a short period of time. For this case reactor is jacketed to add more heat by supplying heat from steam boiler through the reactor wall. This steam is generated by burning of jatropha cake in fire tube boiler. The main consideration of using this heat transfer by steam instead of direct heating of electric energy; is to recover the residue left from extraction of jatropha oil from the seed and kernel. This system is integrated to the system and the insulator is covered on the jacket to prevent heat loss from the internal system to the surrounding. The fire tube boiler is used for the generation of steam energy by burning of biomass of jatropha cake. Mainly to generate energy from biomass is a renewable source of energy.

### **2.8.2. Application of Fire Tube Steam boiler for heating of batch reactor**

Steam is the current energy sources of the industry worldwide. It is used in the production of food, equipment process, cooling and heating of large buildings, and production of electricity. Steam boiler is a closed vessel which usually generates steam from water by combustion of fuel [43]. Therefore, steam is a crucial area of study in energy generation in many engineering areas. Steam boiler have two parts ,combustion chamber where the fuel is burned and heat exchanger which transfer heat to water from the combusted fuel[44]. Boiler types comprises of water tube, fire tube, modular, coil tube. Fire tube boilers are safer to use, needs lesser experts, and works under low pressures than water tube boiler. Therefore, it can be used in small application areas. On the other hand, Water tube boilers have high steam production rate ,easily transported and constructed[43]. They are designed to withstand the stress [45]. In boilers heated water, steam is generated or superheated , under pressure or vacuum by the application of heat generated from the combustion of fuel (such as natural gas ),electrical heating system and recovery and conversion of normally unused fuel [46]. Many different solids, liquids and gaseous fuel are fired in boiler. Fuels such as biomass ,fossil fuel, and refuse derived fuel as well as other fuels and fuel combinations are used for [47].

## **2.9. Selection of reactor system for Jatropha oil**

In the case of thermodynamics, the designer can investigate the nature of the reaction heat and whether the reaction is reversible or irreversible. If the exothermic reactions are irreversible, attention may be focused on the influence of reactor design on conversion and heat transfer control. An objective of reactor design is to determine the size and type of reactor and mode of operation for the required job. The choice of reactors depends mainly on the safety, environment, and profit. Optimization techniques are often employed during the design stage to establish the optimum design from the profit viewpoint. This includes factors such as raw materials, initial and operating costs, and the market value of the finished products. The designer also requires knowledge of reactor performance before reviewing an optimization technique. Chemical reactions are performed in reactor systems that are derived from one of the following basic types of model reactors:

- The well-mixed reaction system with uniform composition that is operated batch wise.
- The semi batch reactor where the incoming and outgoing mass flows are not equal to each other and the total mass of the reacting mixture is not constant.
- In continuously operated stirred tank reaction the composition of the reaction mixture is assumed uniform and equal to the composition at the outlet.
- The tubular (plug flow) reactor in which piston flow of the reacting mixture is assumed, and there is neither mixing nor diffusion in the flow direction.

Batch reactors can be categorized in several different ways according to: Equipment (tank, tube, and tower), the reaction system (homogenous or heterogeneous, liquid, gas or solid phase), Temperature control (isothermal or adiabatic) and Mode of operation (batch wise, semi batch or continuous). There are three types of heads.

- Ellipsoidal head
- Torrispherical head
- Hemispherical head

### **2.9.1. Jacketed vessel or jacketed batch reactor**

The most commonly used type of jacket is consisting of an outer cylinder that surrounds part of the vessel. The heating or cooling medium circulates in the annular space between the jacket and vessel walls, and the heat is transferred through the wall of the vessel. Circulation baffles are usually installed in the annular space to increase the velocity of the liquid flowing

through the jacket and improve the heat transfer coefficient. The same effect can be obtained by introducing the fluid through a series of nozzles spaced down the jacket. The momentum of the jets issuing from the nozzles sets up a swirling motion in the jacket liquid. But, the simple jacketed cylinder of the reactor is feasible for small heat transfer rate which is for heating purpose of the reactants in the reactor. This is mainly to speed up of the reaction rate and to reduce the retention of chemical reaction. The spacing between the jacket and vessel wall will depend on the size of the vessel but will typically range from 50 mm for small vessels to 300 mm for large vessels. Conventional jacketed heat exchanger and its heat transfer process can be considered as a parallel plate heat exchanger channels. The velocity of the fluid is parallel to the wall, so the angle between the velocity vector and the temperature gradient close to  $90^\circ$ . If the coordination degree of velocity and temperature fields is inadequate, so is the heat transfer performance[43- 45].

### **2.9.2. Factors influencing agitation**

Agitation of the vessel reactor is affected depending on the following cases. These are: - Mass transfer at an interface, Heat transfer at an interface, Dispersion of solids, liquids or gases. The factors which influence the rate and degree of mixing as well as the efficiency may however be classified as follows:

- Characteristics concerned with the rotating impeller e.g. its shape, speed, dimensions and position in the vessel.
- Physical properties of the materials concerned. E.g. their densities, viscosities and physical states.
- Shape and dimensions of the containing vessel end of any fitting which may be immersed in the fluid

Agitation is mainly completed by the rotation of shaft and impeller rotation during mixing and speeds up of chemical reaction[51]. For this case appropriate impeller type is needed. Impeller selection can be depending on the following flow properties: Laminar flow and turbulent flow, and depends on the flow pattern.

For the laminar flow of fluid, the impeller size is large and it may be equal to the size of the vessel wall. Since laminar flow does not transfer momentum as turbulent flow, laminar flow impellers must be largest to affect the desired physical, chemical and transport results throughout the tank.

There are three main types of flow pattern. These are:-

i. Axial mixing flow

The fluid flow is parallel to the axis of rotation; it moves media from the top to the bottom. Axial flow impellers are used for blending, solid suspension, solid incorporation or draw down. It is mostly common in low viscosity, high speed application. The most common impeller style is the propeller.

ii. Radial mixing flow

The fluid is discharged radially outwards to the vessel wall. Compared to axial flow impellers, radial flow impellers provide high shear and turbulence levels with lower pumping. A radial flow draws the media from the top bottom. They are used for liquid dispersion for low to medium viscosity fluids and high speeds. The most common impeller styles are the straight blade and cross blade.

iii. Tangential mixing flow

The flow pattern seen when the tangential or rotational flow dominates, swirling of the tank contents often with surface vortex. It is often used when mixing high viscosity at lower speeds. Most impeller styles are U-shaped anchor and square blade impeller. Anchor and helix impellers are for liquids of very high viscosity [52]. In these liquids, the agitation process is under laminar flow conditions, and unusual impeller shapes, such as the anchor, the helical ribbon, the screw impeller, or some other similar shapes are most satisfactory. Many non-Newtonian solutions, usually having a high viscosity, are agitated with these types of impellers.

Table2. 5. Fuel properties of mineral diesel, Jatropha biodiesel, Jatropha oil

Application	Power(W/m <sup>3</sup> )
Blending <sup>a</sup>	39.4-98.5
Homogeneous Reaction <sup>a</sup>	98.5-295.5
Reaction with Heat Transfer <sup>a</sup>	295.5-985
Liquid-Liquid Mixtures <sup>a</sup>	985
Liquid-Gas Mixtures <sup>a</sup>	985-1970
Slurries <sup>a</sup>	1970
Fermentation <sup>b</sup>	591-1970
Emulsion Polymerization <sup>b</sup>	1182-1379
Suspension Polymerization <sup>b</sup>	591-1970
Solution Polymerization <sup>b</sup>	2955-7880

a)Source: Reference[53]

b) Source: Reference [55]

The simplest method for producing ethyl esters is to use a batch, stirred tank reactor. Alcohol to glyceride ratios from 4:1 to 20:1 (mole: moles have been reported, with a 6:1 ratio are most common). The operating temperature is usually 65<sup>0</sup>C, although temperatures from 25<sup>0</sup>C to 85<sup>0</sup>C have been reported. The most common used catalyst is sodium hydroxide, with potassium hydroxide is used. Typical catalyst loadings range from 0.3% to about 1.5%. Thorough mixing is necessary at the beginning of reaction to bring the oil, catalyst and alcohol into intimate contact. Towards the end of the reaction, less mixing can help increase the extent of reaction by allowing the inhibitory product glycerol to phase separate from ester-oil phase. Completions of reaction from 85% to 94% are reported. Some groups use a two-step reaction, with glycerol removal between steps to increase the final reaction extent to 95%. Higher temperatures and higher alcohol: oil ratios also can enhance the percent completion. Typical reaction times ranges from 20 minutes to more than one hour[54]. The oil is first charged to the system, followed by the catalyst and methanol. The system is agitated during the reaction time, and then the agitation is stopped.

The use of computers to solve the fluid flow and heat transfer related problems is referred to as computational fluid dynamics or in abbreviated form as CFD. The accuracy of results of numerical solution of transport phenomenon problem by CFD analysis is often debated in

comparison to the experimentally obtained results[55]. However, if the solution approach of CFD analysis is such that it is based on accurate problem set-up and computational procedure, then the results can be treated with reasonable accuracy comparable to the experimentally obtained values. But again, this strongly depends on the CFD user's knowledge in defining the problem and performing simulations. The advantages of choosing CFD analysis over experimental study are: a) CFD analysis is often inexpensive b) Parametric studies with different variables can be done with ease c) The problem can be simplified by assumptions.

A common discretization scheme utilized in CFD analysis is the Finite Volume Method, which is based on dividing the computational domain into control volumes. The differential equations are integrated over the control volumes and divergence theorem is applied. To evaluate the derivatives, the values at the control volume faces are required, which is based on some assumption about its variation. The result is a set of algebraic equations one for each control volume which is solved iteratively. In the present work, ANSYS Fluent software package was used for CFD analysis which is based on Finite Volume Method[56]. Fluent is a commercial CFD package, which can be used to solve Navier-Stokes equations using Finite-Volume methods[57].

## CHAPTER THREE

### MATERIALS AND METHODOLOGY

#### 3.1. Materials

Jatropha oil and Jatropha cake ,Dehydrated Ethanol i.e. around 99.8% of water content, Sodium hydroxide catalyst, jacketed batch reactor, Furnace, Jatropha cake boiler, Thermal insulation i.e. phenolic foam.

#### 3.1.2. Material selection

The selection of a proper material, for engineering purposes, is one of the most difficult problems for the designer. The best material is one which serves the desired objective at the minimum cost. The following factors should be considered while selecting the material:

- Availability of the materials,
- Suitability of the materials for the working conditions in service, and
- The cost of the materials.

The important properties which determine the utility of the material are physical, chemical and mechanical properties. Stainless steel material is selected for the construction of reactor. The cylindrical nature of mixing is selected for facilitating mixing of reactants.

Table3.1. Physical properties of metals[58]

Metal	Density (kg/m <sup>3</sup> )	Melting point (°C)	Thermal conductivity (w/m°C)	Coefficient of linear expansion at 20°C (µm/m/°C)
Aluminum	2700	660	220	23.0
Brass	8450	950	130	16.7
Bronze	8730	1040	67	17.3
Cast iron	7250	1300	54.5	9.0
Copper	8900	1083	393.5	16.7
Lead	11400	327	33.5	29.1
Monel metal	8600	1350	25.2	14.0

Metal	Density (kg/m <sup>3</sup> )	Melting point (°C)	Thermal conductivity(w/m <sup>0</sup> C)	Coefficient of linear expansion at 20°C (µm/m/°C)
Nickel	8900	1453	63.2	12.8
Silver	10500	960	420	18.9
Steel	7850	1510	50.2	11.1
Tin	7400	232	67	21.4
Tungsten	19300	3410	201	4.5
Zink	7200	419	113	33.0
Cobalt	8850	1490	69.2	12.4
Molybdenum	10200	2650	13	4.8
Vanadium	6000	1750	-	7.75

### 3.1.3. Material selection for simple jacket

#### 1. Purpose

The stainless steel tank also called steam jacket tank, is widely used for candy, pharmacy, dairy, wine, beverage, tin can and food process, can be used also for large restaurant cooking. It is good equipment during food processing to improve quality, shorten time, and improve working conditions.

#### 2. Features

This tank is used at a certain pressure steam as the heating source, with big heating area, high heat effect, heating evenly, liquid material boiling time is short, and the heating temperature is easy to control. The inner tank material adopts imported resistance in stainless steel manufacture, equipped with pressure meter, safety valve, easy to install and operate, safety and reliable.

### 3.2.2. Selection of material for steam boiler

For selection of boiler, the knowledge of material available and the properties they possess are very important. For choosing of the material for the fire tube boiler, we shall consider the following factors which affect the choice of material selected and used for the design of the boiler type.

1. The suitability of the material for the working conditions in service, considering characteristics such as; appearance, thermal conductivity, rate of emissivity, strength, stiffness, creep, etc.
2. Availability of the material: the ease at which the materials are seen or purchased in the market.
3. Workability of the material: considering possible methods of processing material selected into desired shape such as; weld ability, machinability, formability, and workability.
4. Expected load or force as well as adequate strength in conformity so as to function satisfactorily without failure.
5. Cost of the material (economic consideration).

#### Material choice

- Furnace, fire- tubes, return chamber and smoke stack: stainless steel; affordable, available, weld able, malleable, strength, high conductivity, and corrosion resistance
- Pressure vessel: Steel; low cost of fabrication, stronger, quick weld ability, cheaper and less labor.

### **3.2. Methodology**

#### **3.2.1. Selection of stirred batch reactor**

The operating mode of jacketed batch reactor may be either continuous or batch. A jacketed batch reactor consists of a vessel to contain the reactants, a jacket, a mixer, and baffles to prevent vortex formation and to increase turbulence, enhancing mixing. To evaluate and select a jacketed reactor, consider the following factors:

- Mixing
- Heat transfer
- Jacket pressure drop
- Cleaning

Sufficient power is needed to mix the liquid to the approach of ideal model throughout the mixing of the liquid. If inadequate mixing is taking place, it will result in the longer residence time and the larger reactor volume than the ideal model. In designing the mixing system requires selecting and sizing of impeller, and baffles. An important consideration of reactor designing is the heating or cooling the reactor contents. To heat the reactor, external

or internal heat exchanger is used. The internal heat exchanger is applied directly to the fluid mixed directly. These heat exchangers are spiral coils, harp coils and hollow or plate baffles.

The external heat exchanger was jacketed or a shell and tube heat exchanger. The jacket types consist of the simple jacket with or without a spiral baffle or nozzles for promoting turbulence- the partial pipe coil, and the dimple jacket. The jacket consists of an outer cylinder enclosing part of the reactor. The heat transfer fluid is flowing through the annular area surrounding the reactor. If the heat transfer rate is limited by the jacket heat transfer coefficient, then increase in turbulence in the jacket by using spiral baffle or nozzles. The jacket area covers about 80% of the reactor surface, consisting of a bottom conical head and a cylindrical shell. The factors that influence the selection of a heat exchanger are:

- Heat transfer coefficient
- Jacket pressure
- Reactor pressure
- Jacket pressure drop
- Cleanliness
- Cost

The jacket pressure and reactor pressure also influences jacket selection. If the jacket pressure is large the reactor wall thickness becomes large, reducing heat transfer [59].

Table 3.2: Chem. Eng.et al.,[59] has given the following rules for selecting the jacket type.

For $\leq 1.8m^3$	Use simple jacket
For $> 1.8m^3$	Use dimple or half-pipe coil
If the reactor pressure is greater than twice the jacket pressure	Use the simple jacket
For jacket pressure $\leq 300psi(20.7bar)$	Use the dimple jacket
For a jacket pressure $>20.7bar$	Use half pipe coil jacket
But $<68.9 bar$	Use half-pipe coil jacket
For steam the pressure is $\leq 51.7bar$	Use the half-pipe coil

This operating mode is unsteady state. The other unsteady state reactors are:

1. Continuous addition of one or more reactants with no products withdrawal and
2. All the reactants added at the beginning with continuous withdrawal of product.

At steady state, reactants flow into and products flow out continuously without a change in concentration and temperature in the reactor. Generally, if residence time is large and the production rate slow, select a batch reactor. Ansys fluent Release 17.2 has been used to develop a finite volume analysis. The transesterification reaction has not been taken into account in the current simulation scenario, but its implementation will be considered in future works to analyze chemical composition changes while a reaction takes place.

## CHAPTER FOUR

### DESIGN ANALYZING OF REACTOR HEATED BY STEAM BOILER

#### 4.1. Sizing of batch reactors

The reactor volume is greater than the reaction volume because of an allowance for head space. To design the reactor of the chemical process, the following procedure is followed.

1. Calculate the volume of reactor
2. Calculate the heat transfer area

Table 4.1: Standard Stirred Tank Reactors source Ref.[60]

Rated Capacity m <sup>3</sup>	Actual Capacity m <sup>3</sup>	Jacket Area m <sup>2</sup>	Reactor Outside Diameter m	Reactor Height (H) m
1.8925	2.11	6.97	1.37	1.29
2.839	3.05	9	1.52	1.52
3.785	4.1	10.96	1.68	1.68
4.542	4.74	12.5	1.68	1.98
5.678	5.9	14.4	1.90	2.05
7.570	7.9	17.74	1.98	2.4
9.463	10.43	21.37	2.13	2.7
11.355	12.38	23.8	2.3	2.7
13.25	14.49	26.3	2.43	2.82
15.140	16.48	28.2	2.59	2.82
22.710	24.98	36.7	3.04	3.05
30.280	33.18	43.3	3.4	3.35
37.85	40.78	50.2	3.7	3.35

#### 4.2. Calculation of reactor unit

The operational volume of the reactor is assumed to be  $V=150L$  and assume that  $H/D$  is taken as 1.5. Sizing of the reactor is done by using the following equation [61]:

$$V = \frac{\pi \times D^2 \times (1.5 \times D)}{4} \quad (4.1)$$

$$V = \frac{\pi \times 1.5 \times D^3}{4}$$

$$D = \sqrt[3]{\frac{4 \times V}{1.5 \times \pi}} \quad (4.2)$$

$$D = \sqrt[3]{\frac{4 \times 0.150}{\pi \times 1.5}} \approx 0.5m$$

$$\frac{H}{D} = 1.5$$

$$H = 1.5 \times D = 1.5 \times 0.5 = 0.75m$$

The area of heat transfer;

$$A = \pi DH = \pi \times 0.5m \times 0.75m$$

$$A = 1.1775m^2$$

The volume of the jatropha oil and ethanol with catalyst filled should be 75% of the reactor to avoid splashing of the reactants[62]. Therefore, the volume of reactant in the reactor will be:

$$0.75 \times 150 = \mathbf{112.5L}$$

Height of the dished bottom is assumed =0.2m. Therefore, the total height =0.75+0.2=0.95m

### 4.3. Designing condition for reactor vessel

#### Pressure determination

According to standard, design pressure (internal pressure) should be equivalent to pressure set for relief valve. Atmospheric pressure is assumed as 102.7kPa (this is atmospheric pressure of Addis Ababa); and hydrostatic pressure is calculated from the following equation:

$$\text{Hydrostatic pressure, } Ph = \rho hg$$

Nasim et al,2013 [63], Assuming the feed stock density as  $920 \frac{kg}{m^3}$  and H=950mm

Where H is stands for the height of chemical reactor,

$$P_h = \rho g H$$

$$P_h = 0.95 \times 920 \times 9.81$$

$$P_h = 8.573 \text{ kPa} \approx 9 \text{ kPa}$$

As per standard, designed pressure is calculated as,

$$P_d = P_h + P_g \quad (4.3)$$

$$P_d = 9 + 102.7$$

$$P_d = 111.7 \text{ kPa} \approx 112 \text{ kPa}$$

Maximum allowable pressure =  $1.33 \times 112 \approx 149 \text{ kPa} = 1.5 \text{ bar}$

#### Wall thickness design

$$\text{Wall thickness} = \frac{p \times r_i}{SE_j - 0.6p} + C_c \quad (4.4)$$

✚ Material for reactor design = stainless steel

⊕ Working pressure of stainless steel,  $S = 94408 \text{ kN/m}^2$ , Joint efficiency,  $E_j = 0.85$

Internal radius =  $0.25 \text{ m}$ , corrosion allowance =  $2 \text{ mm}$

$$\frac{P \times r_i}{SE_j - 0.6p} + C_c = \frac{149 \text{ kPa} \times 0.25 \text{ m}}{94408 \text{ kPa} \times 0.85 - 0.6 \times 149 \text{ kPa}} + 0.002 \text{ m}$$

Therefore, wall thickness =

$$t_{\text{wall}} = \frac{37.25}{80157.4} + 0.002 = 0.0025 \text{ m} = 2.5 \text{ mm} \approx 5 \text{ mm}$$

Outside diameter =  $D_i + 2t = 0.5 \text{ m} + 2 \times 0.005 \text{ m} = 0.510 \text{ m}$

#### Reactor head

The maximum allowable pressure designed for the selected reactor is 1.5 bars. That is why we have selected a Torrispherical head.

$$t_H = \frac{1.104 P_D}{2 \times \varepsilon H_s - 0.2p} + t_c = 0.0025 + 0.002 = 0.0045 \text{ m} \approx 5 \text{ mm}$$

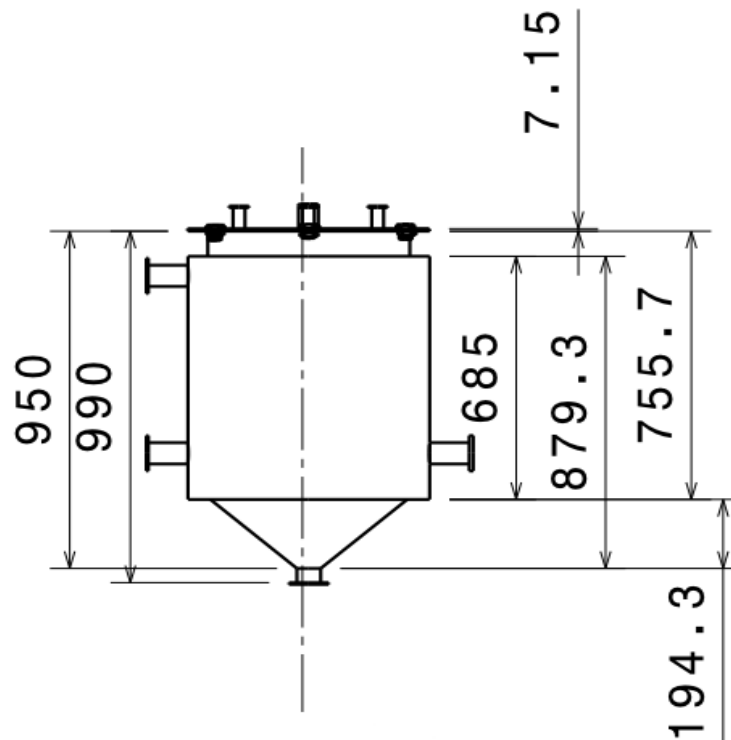


Figure 4.1: over all dimensions of Batch reactors with jacketed heat exchanger

#### 4.3.1. Determination of temperature for biodiesel formation

Transesterification reaction is takes place from 60-120 temperature range[64]. Maximum operating temperature of reactor vessel was taken as 85 with 10 °C allowance. Therefore, the maximum design temperature of the reactor vessel is 80°C which is facilitating in design of heating element. In this research work steam boiler which is used to heat the vessel through jacketed vessel. The thickness and material of jacketed and reactor is selected accordingly. We have two different reactors which have the volume equal to 150 L. The volume of reactant should be filled about 75% of the container. Therefore, the volume of the reactant is 0.1125m<sup>3</sup>. From standard table Chem. Eng.et al.,[59], for  $\leq 1.89\text{m}^3$  we must use simple jacket for heat exchanging purpose. The maximum designed allowable pressure for the reactor is 1.5 bars. This pressure is the summation of the atmospheric and internal pressure applied on the reactor. At 1.8m<sup>3</sup> reactor volume, the jacketed area is equal to 6.9m<sup>2</sup> from the standard. From this we can find the diameter of the jacket equal to 2.98m. From this standard, the diameter and the height of the reactor are 1.37m and 1.295m respectively. From the size of our reactor, we can assume the jacket diameter as 0.60m by relying on the standard diameter of the jacket. The gap between the reactor and the jacket will vary from 50mm and 300mm for small and large reactor respectively. The small gap between the

jacket and reactor is used for efficiency of heat transfer during heating of the chemical reaction.

By having this diameter, the cross sectional area of the jacket is:

$$A = \frac{\pi \times (D_2^2 - D_1^2)}{4} = \frac{\pi \times (0.6^2 - 0.5^2) m^2}{4}$$

$$A = 0.0864 m^2$$

The jacket cross sectional area needed for heat exchanger during heating of 0.15m<sup>3</sup> reactor tanks to heat jatropha oil from 25°C to 80 °C is  $\pi DH = \pi \times (0.60 \times 0.75) m^2 = 1.413 m^2$

#### 4.3.2. Impeller calculation

The design of agitator is given in standard design from Houston, Texas, 2001 [61] as the following formulas.

Agitator dimensions are:

Impeller diameter,  $D_a = D_t/3 = 0.5/3 = 0.17m$  (4.5)

Impeller height above vessel floor,  $E = D_a = 0.17m$

Length of impeller blade,  $L = D_a/4 = 0.17/4 = 0.043m$

Width of impeller blade,  $w = D_a/5 = 0.034m$

Number of impeller = 2

Number of impeller blade = 6

Distance between consecutive impellers = 0.17m

Assume that the rotational speed of the tip impeller is 300rpm[65],

Tip velocity =  $\pi \times D_a \times N = \pi \times 0.17 \times 300rpm$   
 $= \pi \times 0.17m \times 5/sec$

$$V = 2.670 \frac{m}{sec} \cong 3 \frac{m}{sec}$$

From standard tip velocity is 3-6 m/s. Therefore, tip velocity of impeller is equal to 3m/s.

### 4.3.3. Power calculation

The difference in the tips velocities between layers of fluids leads to shearing action within the layers, thus causing molecular separation. The high velocity streams on the walls of the reactor causes molecular separation.

Let assume rotational speed  $N=300-350$  rpm and  $0.920$  g/ml of jatropha oil,

$$F = mrw^2. \quad (4.6)$$

$$F = mr \times (2\pi n)^2$$

$$\rho = \frac{m}{v}$$

$$m = \rho \times v$$

$$m = 920 \frac{\text{kg}}{\text{m}^3} \times 0.1125 \text{m}^3$$

$$m = 103 \text{kg}$$

$$F = 103 \times 0.25 \times \left( \frac{2\pi \times 300}{60} \right)^2$$

$$F = 26.65 \text{kN}$$

The power consumed by an agitator at various rotational speeds and physical properties (e.g. Viscosity and density) for a system's geometry can be determined from the power number correlation. The procedure involves:

- Calculating the Reynolds number  $N_{Re}$  for mixing
- Reading the power number  $N_p$  from appropriate curve, and calculating the power  $P$  given by:

$$P = \rho \times N_p \times N^3 \times Da^5 \quad (4.7)$$

$$N_{Re} = \frac{N \times Da^2 \times \rho}{\mu} \quad (4.8)$$

Nasim et al.,2013[63],Where;  $N = 300$ rpm,  $Da = 0.17$ m,  $\rho_{\text{jatropha oil}} = 920$  kg/m<sup>3</sup>, viscosity ( $\mu$ ) =  $0.0331$ kg/ms and  $g_c = 9.8$  m/s<sup>2</sup> (constant gravity).

$$N_{Re} = \frac{300/60 \times (0.17)^2 \times 920 \left( \frac{r}{s} \times m^2 \times \frac{\text{kg}}{m^3} \right)}{0.0331} \Bigg/ \text{kg/ms}$$

$$N_{Re} = 4016.314$$

By having this Reynolds number and reading the  $N_p$  from appropriate curves for flat blade disk turbine,  $N_p = 4.5$  [66].

Power number ( $N_p$ ) = 4.5

Shaft rpm ( $N$ ) = 300rpm = 5rev/sec

$$P = N_p \times N^3 \times Da^5 \times \rho$$

$$P = 4.5 \times (5)^3 \times (0.17)^5 \times 920 \left( \frac{\text{rev}^3}{\text{s}^3} \times \text{m}^5 \times \frac{\text{kg}}{\text{m}^3} \right) \left( \frac{\text{rev}^3}{\text{s}^3} \times \text{m}^5 \times \frac{\text{kg}}{\text{m}^3} \right) = \text{kg} \times \frac{\text{m}}{\text{s}^2} \times \text{m} \times \frac{1}{\text{s}} = \frac{\text{Nm}}{\text{s}} = \frac{\text{J}}{\text{s}}$$

$$P = 73.5\text{w}$$

$$1\text{w} = 0.00134\text{hp}$$

$$P = 73.5 \times 0.00134\text{hp}$$

$$P = 0.10\text{hp}$$

Now assuming the impeller is 85% efficient:

Actual power required =  $86.5\text{W} = 0.103/0.85 = 0.121\text{hp}$

Studies on various turbine agitators have shown that geometric ratio that deviate from standard design causes different effects on the power number  $N_p$  in the region turbulent [67].

- For the flat, six –blade open turbine,  $N_p \propto (W/Da)^{1.0}$
- For the flat, six blade open turbine, varying  $Da/DT$  from 0.25 to 0.5 has no effect on  $N_p$
- When two six-blade open turbines are installed on the same shaft and the spacing between the bottom edges of the two turbines) is at least equal to  $Da$ , the total power is 1.9 times a single flat-blade impeller.

For the two impellers, the power required is calculated as follows:

$$P = P_a \times 1.9$$

$$P = 86.5 \times 1.9$$

$$P = 164.35\text{w}$$

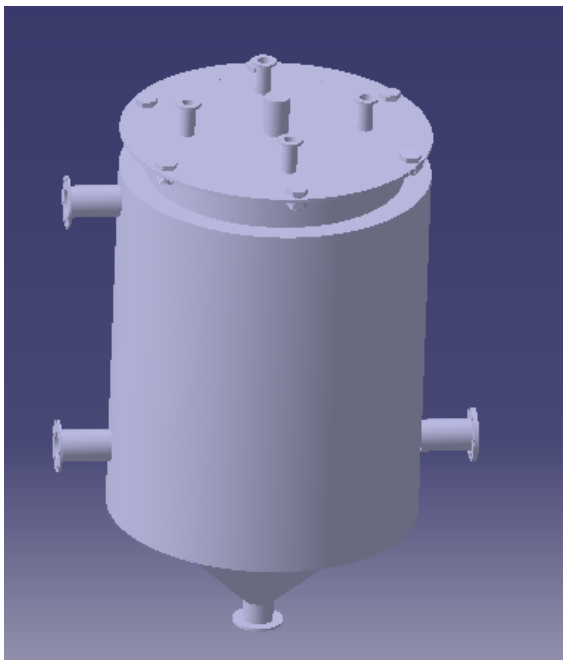
### **Baffle design**

Number of baffles = 4

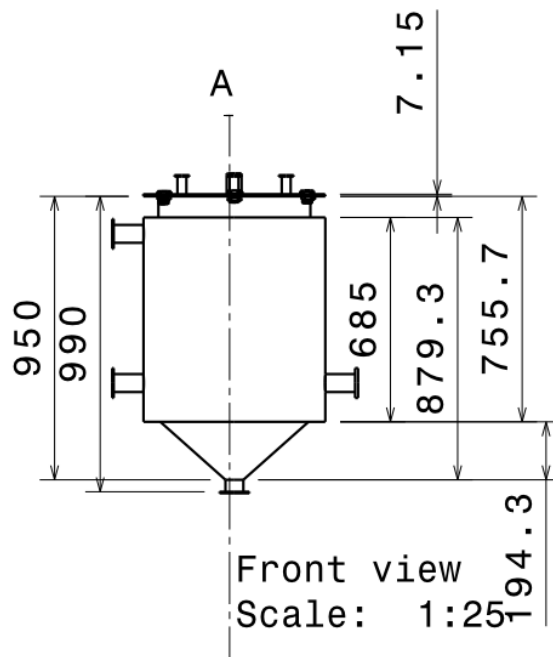
Width of one baffle =  $Dt/10 = 0.50/10 = 0.05\text{m}$

(4.9)

Height of baffle =height of reactant=0.75m



(a)



(b)

Figure4.2: (a) represents 3D of assembled jacketed agitated reactor, (b) over all dimensions of jacketed agitated reactor

#### 4.3.4. Analyzing the amount of steam generated from jatropha boiler

The mass of jatropha seed and knells used for the extraction of jatropha oil is 150 kg within 150L of batch reactor. By solvent extraction, 50% of jatropha oil is extracted from seed and knells. From this extraction, 50% of jatropha cake is formed. This jatropha cake mass will be 75kg within 19783.6kJ/kg gross calorific value and 75 kg of jatropha oil will be extracted. This jatropha cake is burned in fire tube boiler to generate steam required for heating batch reactor.

The combination of shell and EFB (empty fruit bunch) 75kg with average GCV of 19783.6kJ/kg produced 95°C steam temperature at 8 min of the firing time. The capacity of the boiler is to produce 95°C and 1.5 bar pressure. The mass flow rate of water is 1877.96kg/hr into water drum of fire tube boiler. The amount of heat ( $Q_t$ ) required during the burning of 75 kg jatropha cake at the expected pressure and temperature is given by[68]:

$$Q_t = Q_s + Q_l \quad (4.10)$$

Where ,

$Q_s$  is the sensible heat

$Q_l$  is the latent heat

$$Q = M_s h_g + M_w C_p \Delta T$$

$$C_p = 4.12 \text{ kJ}$$

The combustion chamber is to house 75 kg of jatropha cake per hour. It was found that the composition of jatropha cake (organic) is 50% C, 6.1 % H and 43.9% (O+N), [69]. The minimum air requirement for incomplete combustion was expressed as  $\left(\frac{8}{3}C + 8H + S\right)$  kg while for complete combustion is  $\left(\frac{100}{28}\right)\left(\frac{8}{3}C + 8H + S\right)$  kg [70]. Substituting values of C, H and S, the minimum value of air required was found to be 6.01 kg and for incomplete combustion 1.1 kg.

Therefore, the amount of heat required to produce the steam at the given pressure by burning of jatropha cake will be the following calculation. The gross calorific value of jatropha cake is 4725 kcal/kg = 19783.6 kJ/kg [71].

$$\dot{m}_f = \frac{Q}{GCV} \quad (4.11)$$

Heat input during the burning of jatropha cake in the fire tube boiler is calculated from the following relation Geankoplis et al., 2003 [72].

$$Q = \dot{m}_f \times GCV$$

$$Q = 75 \frac{\text{kg}}{\text{hr}} \times 19783.6 \frac{\text{kJ}}{\text{kg}}$$

$$Q_{in} = 1483770 \frac{\text{kJ}}{\text{hr}} = 412.16 \text{ kW}$$

The mass flow rate of steam is calculated by rearranging equation (4.10),

$$\dot{m}_s = \frac{Q - M_w C_p \Delta T}{h_g}$$

$$\dot{m}_s = \frac{412.16 - 1877.96 \times 4.12 \times (95 - 30)}{2667.6}$$

$$\dot{m}_s = \frac{(412.16 - 139.7)kW}{2667.61(kJ/kg)}$$

$$\dot{m}_s = 0.102 \frac{kg}{s}$$

$$\dot{m}_s = 367 \frac{kg}{hr}$$

Therefore the Boiler capacity is 367 kg/hr.

The efficiency of boiler is calculated from Hussain et al.,2003 [73] relation below,

$$\eta_b = \dot{M}_s \times \frac{(h_g - h_f)}{\dot{M}_f \times C_v} \times 100\% \quad (4.12)$$

The value of saturation steam enthalpy and feed water enthalpy is read from steam table at the designed pressure of boiler as follows.

$h_g@95^\circ C = 2667.6kJ/kg$ ,  $h_f@30^\circ C = 125.74kJ/kg$

$$\eta_b = 367 \times \frac{(2667.6 - 125.74)}{75 \times 19783.6} \times 100\%$$

$$\eta_b = \frac{93286262}{14837700} \times 100\%$$

$$\eta_b = 62.9\%$$

Due to its high calorific value of jatropha cake, the efficiency of this boiler is approximately 63%.

## CHAPTER FIVE

### MODELING OF HEAT TRANSFER IN JACKETED BATCH REACTOR

Batch processes are used extensively in the manufacture of relatively small volume products with relatively high value. This production is used to multi-purpose production. The achievement of stable and reproducible operating conditions is important in order to achieve the required product purity, yield, and relevant regulatory authorities. Batch processes are inherently transient in nature and the capability to demonstrate dynamically the adequacy of equipment design and performance provides a powerful design tool. Dynamic modeling can prevent costly mistakes prior to start up. Once a process model signature has been validated against real plant performance the dynamic model can be used as a diagnostic tool to identify operating problem. Many stirred tank bioreactors and chemical reactors require precise control of both mixing and heat transfer to achieve optimum productivity [74]-69]. Heat transfer in agitated vessels is one of the most significant factors for controlling the outcome of biochemical processes. The temperature of fermentation generally must be maintained within very narrow limits [76]. Usually, agitated vessels have a heat transfer surface, in the form of a jacket or internal coils, for addition or removal of the heat. The intensity of heat transfer during mixing of fluids depends on the type of the agitator, the design of the vessel and conditions of the process.

When designing an agitated vessel, the impeller, vessel geometry and baffles should give the degree of mixing the process demands, but it is impractical to specify the agitator to give a specific heat transfer coefficient. The main factor when selecting an agitator is the nature of the fluid. Large diameter agitators operating at low speeds normally give excellent blending and heat transfer characteristics with high viscosity fluids. Small impellers operating at high speed are more suited for low viscosity fluids. Turbine impellers are normally used for high speed, low viscosity applications. The normal design of turbine impeller has either four or six flat blades on a central disc. The ratio of turbine diameter to vessel diameter  $d/D$  is usually in the range from  $1/3$  to  $2/3$ . Baffles are essential in stirred batch vessels to provide good mixing patterns throughout the vessel. They act to reduce tangential flow and promote axial motion. As baffling increases turbulence, it affects the heat transfer rates. Because heat transfer in agitated vessels is complex, an empirical approach based on dimensionless analysis has been used to predict the average heat transfer coefficients at the jacketed wall.

Hence, the results of many heat transfer studies are frequently correlated using a dimensionless equation.

$$Nu = \Theta_{10} Re^{\Theta_{20}} Pr^{\Theta_{30}} V_i^{\Theta_{40}} \quad (5.1)$$

Where;  $\Theta_{10}$ ,  $\Theta_{20}$ ,  $\Theta_{30}$ , and  $\Theta_{40}$  are found by fitting equation (5.1) to experimental data. A review of many such correlations has been presented by Experimental Thermal and Fluid Science 5, [77]. Extensive characterization work has been carried out by authors for different agitator types. The values of the constant  $\Theta_{10}$  reported are given in Table 5.1.

Table5.1: Exponent for different impellers and Re regimes

Type of agitator	Re range	$\Theta_{10}$
Flat blade disk turbine		
Unbaffled vessel	Re<400	0.54
Baffled vessel	Re>400	0.74
Propeller with three blades and baffled vessel	5500 to 37000	0.64

The typical values for  $\Theta_{20}$ ,  $\Theta_{30}$  and  $\Theta_{40}$  are respectively 2/3, 1/3 and 0.14 from Chem. Eng. [78]. From the above relations and flat blade disk turbine with baffles, equation (5.1) above can be modified to the following equation.

$$Nu = 0.74Re^{2/3} Pr^{1/3} V_i^{0.14} \quad (5.2)$$

Where;

$$v_i = \mu / \mu_w$$

$\mu$  =viscosity for the bulk of fluid

$\mu_w$ =dynamic viscosity of fluid at wall

The constant  $\Theta_{10}$  which is used to multiply the whole equation have been reported to range from 0.33 to 1.0, mainly varying due to system geometry and type of impeller. Attempts were made to study batch heat transfer in an agitated jacketed vessel, with a view to developing a design equation to determine film heat transfer coefficient,  $h_o$ , in such vessels. But as the variables influencing the heat transfer coefficient are quite large in number,

complete study covering all the variables could not be made. It is essential to have complete information on the effects of possible variables on the rate of heat transfer and also a general correlation valid over wide ranges of operating conditions for heat transfer coefficients for design and efficient working of the process.

### 5.1. Batch heating and cooling of fluids

Batch reactor assumes that the reactant filled and perfectly homogenized in the reactor. The temperature of the reactor is immediately adjusted to that of the heat transfer steam. Therefore, the chemical reaction takes place at the temperature of heat transfer steam under perfect mixing. The process is stopped as soon as the degree of conversion is achieved.

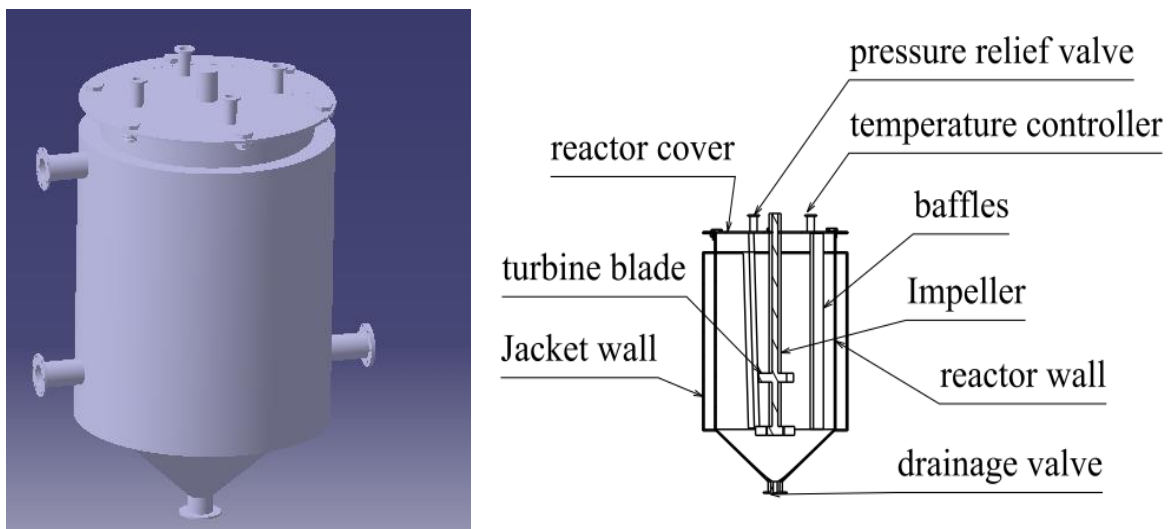


Figure5.1: Assembled jacketed vessel with two inlets and one outlet

Figure 5.1 shows two nozzles at the entrance of reactants and two nozzles for steam inlet and one steam outlet on the side of the jacketed reactor. The batch reactor is extensively used for large scale-up of an industrial plant. The size of batch reactors are ranges from 19L in small industrial pilot plants to 38000-76000L in large plants. When larger sizes are required, the design may include multiple parallel units of reactors. In small industrial pilot plants, we will obtain small quantities of new product for further evaluations such as purity, yield, and sales.

Chemical reaction rates with the temperature and mixing rates. Mechanical agitation promotes the flow of heat by forcing convection of the mass and by reducing the film resistance at the vessel wall. An important purpose of agitation or mixing is to bring a number of materials together in a physically homogenous mixture. Batch reactors are charged with reactants, closed, and heated to reaction temperature, which may be maintained

(i.e. isothermally) for the duration of the reaction. After the reaction is completed, the mixture cooled, and the reactor opened, the product is discharged and the reactor is cleaned for the next batch.

Heating or cooling of process fluids in a batch operated vessel is common in chemical process industries. The process is unsteady state because the heat flow and temperature vary with time at a fixed point. The time required for heat transfer can be modified, by increasing the agitation of batch fluid, the rate of circulation of heat transfer medium in a jacket or heat transfer area. Bondy and Lippa [79] and Dream [80] have compiled a collection of correlations of heat transfer coefficients in agitated vessels. Demerits of batch process because:

- Use of heating or cooling medium is intermittent
- The liquid being processed is not readily available
- The requirements for treating time require holdup
- Cleaning or regeneration is an integral part of the total operating period

The variables in batch heating or cooling processes are surface requirement, time, and temperature. Heating a batch may be by external jacket or coil. In either case, assumptions are made to facilitate calculation ,namely,

- The overall heat transfer coefficient  $U$  is constant for process and over the entire surface
- Liquid flow rates are at steady state
- Specific heats are constant for the process
- The heating or cooling medium has a constant inlet temperature
- Agitation gives a uniform batch fluid temperature
- There is no phase change
- Heat losses are negligible

## **5.2. Methods of Heat transfer in jacketed batch reactor**

Vessels with mechanical impellers are used in chemical reactors (producing polymers, paints, fertilizers, and resins), chemical, petrochemical, food, textile, and other industries, operating as extractors, and storage vessels. Those process needs heating and cooling, these can be provided by jackets, coils and vertical tube baffles, where the heat transfer area is target of overall heat transfer coefficient. The jackets are surfaces of heat transfer

characterized by encompassing the reactor, given that the thermal fluid to move over a large area, especially without specific purpose (rooms) the space between the reactor and jackets. On this equipment heat transfer efficiency is low due to the heat source being in the wall, which proves uneven heating of the fluid in the reactor, besides the physical structure is big. Nevertheless, this system is easy to clean and the data is available on the open literature [81]. The helical coils made of tubes between the impeller center line and the reactor wall. The heat transfer area contact with fluid is high, which increases the heat transfer efficiency; however, the difficulty is the cleaning of the surface due to it is being at the center of the reactor. The spiral coils consist of the wounded tubes generally placed at the bottom of the reactor. They are applied for pumping of viscous fluid for the transport by heating. Spiral coils have as disadvantage the located heat transfer position, fostering uneven heating. The another demerit of the spiral coil is lack of data in the current literature [82].

The three heating surfaces mentioned above need baffle to avoid vortex, which is characterized by the formation of bottle neck by the agitated fluid around the mechanical impeller. The vortex is indicator inefficiency at mixing and low heat transfer, due to the circular and organized stream lines. However, each type of heat transfer surfaces will present parameters for Nusselt's equation particular to each system in which they were determined, in such a way that it is possible to obtain a general model that covers all surfaces for heat transfer in agitated vessels. Heat transfer area of batch reactor is determined by transient energy balance while the continuous process is by steady state operation.

There are two types of heat transfer process. These are direct heat transfer and indirect heat transfer.

### **5.2.1. Direct heat transfer process**

The direct heat transfer is directing hot steam into the reactants to rapidly heat the reactant stored in a tank. The hot steam condenses in the liquid reactants and gives up its condensation heat to the content of the tank. Direct heat transfer can only be used if the heat carrier introduced does not interfere with the composition and concentration of the reactor filling. In indirect heat transfer the heat is transferred from one fluid to another through a boundary (partition) in a heat exchanger. The fluid flows on the two sides of the partition do not mix. In terms of the flow directions of the fluids on both sides of the partition, we

differentiate between parallel flows, counter flow and cross flow. In other words, the fluids either flow in the same direction, in opposing directions or perpendicular to one another.

### 5.2.2. Indirect heat transfer

When the hot fluid is flowing along the partition, it is cooled and gives up heat to the partition. In turn, the heated partition gives up heat to the cold medium flowing along the other side of the partition. This heats up the cold fluid in the reactor. Heat transfer at the partition can be sub-divided into three separate processes:

1. The hot fluid gives up heat to the partition.
2. The partition conducts heat from the hot surface to the cold surface.
3. The partition gives up the heat to the cold fluid.

The temperature curve at the partition is shown schematically in Fig. 5.2. Each of the three heat transfer processes is assigned a temperature difference ( $\Delta T_h$ ,  $\Delta T_p$  and  $\Delta T_c$ ).

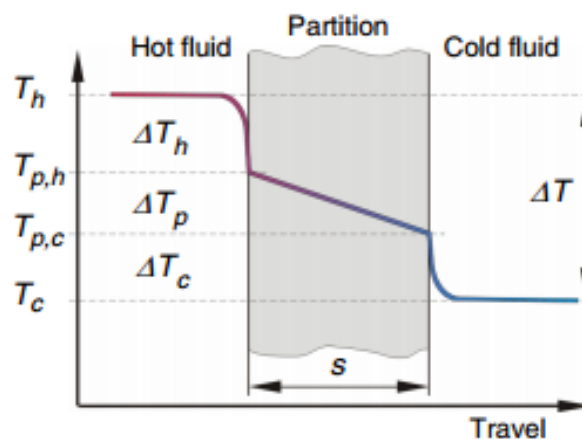


Figure 5.2: Temperature curve at the partition

Where, the variables for the hot side are indicated by the suffix, *h* and those for the cold side with the suffix, *c*. The suffix *p* represents the partition, while the suffixes *in* and *out* indicate the inlet and outlet respectively. The efficiency of a heat exchanger is defined by the quality of the transfer of heat during the three heat transfer processes.

### 5.2.3. Heat transfer from hot side fluid-partition

The ability to transfer heat from one fluid to the partition or vice versa is described by the coefficient of heat transfer, *U* [80].

$$\dot{Q} = U \cdot A \cdot \Delta T \cdot t \quad (5.3)$$

The formula defines the amount of heat  $Q$  transferred in the time  $t$ . As well as the coefficient of heat transfer  $U$  and the partition area  $A$ , the temperature difference between the fluid and partition temperatures is a crucial factor in the heat transfer. In general, the heat flow is the amount of heat per unit time that a heat exchanger transfers. The heat flow is specified using a power unit, e.g. kW or kJ/s. For heat flow the equation is generally:

$$\dot{Q} = U \cdot A \cdot \Delta T \quad (5.4)$$

In the specific case of the hot side of the partition with hot fluid (suffix  $h$ ) or the cold side with cold fluid (suffix  $c$ ):

$$\dot{Q} = U_h \cdot A \cdot \Delta T_h \quad (5.5)$$

Where,  $\Delta T_h = T_h - T_{p,c}$

$$\dot{Q} = U_c \cdot A \cdot \Delta T_c \quad (5.6)$$

Where,  $\Delta T_c = T_{p,c} - T_c$

#### 5.2.4. Thermal Conduction in the Partition

Within the partition the heat is transferred from the hot side to the cold side by **thermal conduction**. Here the following relationship applies:

$$\dot{Q} = \frac{k}{x} \cdot A \cdot \Delta T_p \quad (5.7)$$

Where  $\Delta T_p = T_{p,h} - T_{p,c}$  (5.8)

The  $k$  represents the thermal conductivity of the partition material and  $x$  is the wall thickness of the partition.

### 5.3. Heat transfer analysis of agitated vessel

#### 5.3.1. Heat transfer correlations for agitated fluids

This is used for the process engineer to estimate the overall heat transfer coefficient 'U' that provides the information about the amount of heat to be (5.9) transferred [83].

$$Nu = c Re^a Pr^b \left( \frac{\mu_b}{\mu_w} \right)^c G_c \quad (5.9)$$

$$Vi = \frac{\mu_b}{\mu_w}$$

Where;  $\mu_w$  = dynamic viscosity at the wall

$\mu_b$  = fluid viscosity at the bulk of flow

$G_c$  = geometric correlation factor.

#### **5.4. Heat transfer in agitated reactor**

Agitated vessels with an external jacket or internal coils are increasingly employed in biotechnology and other process applications. The most common type of agitator consists of an external jacket reactor. The heating or cooling medium circulates in the annular space between the jacket and reactor walls. Alternatively, steam is used for heat transfer by heating the liquid in the reactor. Many jacketed vessels are reactors; which is the type of exothermic or endothermic effects. In many applications using jacketed vessels, successive batches of material are heated (or cooled) to a given temperature, and therefore the heat transfer involves an unsteady state process.

##### **5.4.1. Design equation of heat transfer**

Surface area for heating or cooling in agitated vessels is provided by either external jacketing or internal coils (tubular baffles). Jacketing is preferred due to:

- Lesser tendency for fouling
- Cheaper material construction because it does not directly contact with the product
- Easier cleaning and maintenance
- Fewer problems in circulating catalysts and viscous fluids
- Larger heat transfer area

Coils should be considered only if jacketing alone does not provide a sufficient heat transfer area, if jacket pressure exceeds 150psig (10.342 bar), or if high-temperature vacuum processing required.

In the idealized condition, vessels and jackets operate under isothermal situation. Which gives :

$$Q = UA\Delta T \tag{5.10}$$

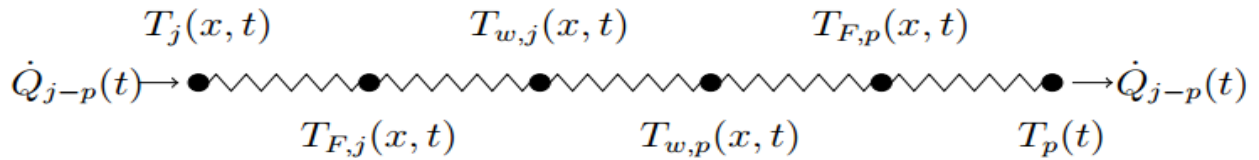


Figure 5.3: Resistance diagram for heat transfer from the jacket to the process

In the realistic continuous situation, where the vessel contents are at constant temperature but, different jacket inlet and outlet temperature [84], equation (5.10) is expressed as :

$$Q = UA\Delta T_{LMTD} \quad (5.11)$$

Where  $\Delta T_{LMTD}$  is the log mean temperature difference between the bulk temperature of the vessel contents,  $t$  and temperature in the jacket,  $T$ .  $\Delta T_{LMTD}$  is expressed as

$$\Delta T_{LMTD} = \frac{(t_2 - T_2) - (t_1 - T_1)}{\ln\left[\frac{(t_2 - T_2)}{(t_1 - T_1)}\right]} \quad (5.12)$$

Where,

$t_1$  = entering fluid temperature in the vessel

$t_2$  = leaving fluid temperature in the vessel

$T_1$  = entering fluid temperature in the jacket

$T_2$  = leaving fluid temperature in the jacket

Under isothermal heat transfer process for heating of batch reactor is,

$$\Delta T_{LMTD} = \frac{T_{b2} - T_{b1}}{\ln\left[\frac{(T - T_{b1})}{(T - T_{b2})}\right]}$$

The over all heat transfer coefficient  $U$  is determined from a series of resistances to the transfer of heat, namely [85].

$$\frac{1}{U} = \frac{1}{h_i} + FF_i + \frac{x_w}{k} + FF_j + \frac{1}{h_j} \quad (5.13)$$

Where

$h_i$  = coefficient of heat transfer area inside the surface of jacketed vessel,  $W/m^2 \cdot ^\circ K$

$FF_i$  = fouling factor inside vessel,  $m^2 \cdot ^\circ C/W$

$x_w$  = wall thickness of vessel ,mm

$FF_o$  = fouling factor inside jacket, $m^2 \cdot ^\circ C/w$

$h_j$  = coefficient of heat transfer area inside surface of jacket, $w/m^2 \cdot ^\circ C$

$k$  = thermal conductivity , $W/m^\circ C$

a) Calculation of inside film ( $h_i$ ) coefficients

When applying the following equations, the calculation of film coefficients in the jacketed vessels, the physical property data should be accurate. This is especially important for the thermal conductivity  $k$ , as its value can have a major impact on the calculated film coefficient and vary widely. The inside film heat transfer coefficient ( $h_i$ ) can be calculated from the following Nusselt number correlation[84]:

$$Nu = C N_{Re}^a N_{pr}^b \left( \frac{\mu_b}{\mu_w} \right)^c \quad (5.14)$$

For agitated vessels,

$$\frac{h_i D_T}{k_f} = C \left( \frac{\rho N D_a^2}{\mu} \right)^a \left( \frac{c_p \mu}{k} \right)^b \left( \frac{\mu_b}{\mu_w} \right)^c \quad (5.15)$$

Where

$h_i$  = heat transfer coefficient to vessel wall,  $w/m^2 \cdot ^\circ C$

$D_A$  = agitator diameter, m

$D_T$  = tank diameter

$N$  = agitator speed (rev/sec)

$\rho$  = density,  $kg/m^3$

$K_f$  = thermal conductivity of the fluid,  $w/m \cdot k$

$C_p$  = specific heat transfer coefficient,  $J/kg \cdot K$

$\mu_b$  = viscosity at bulk fluid temperature,  $kg/m \cdot sec$

$\mu_w$  = viscosity at the wall temperature, kg/m.sec

The value of constant C and the exponents a, b, and c depends on the type of agitator whether baffles are used and their type and whether the transfer is via the vessel wall or to coils. Baffles are used in most applications and the values of a, b and c in the literature are 2/3, 1/3 and 0.14 respectively. To determine the type of agitator used in mixing of jatropha oil at 30°C, the Reynolds number is given as:

$$N_{Re} = \frac{\rho N(d)^2}{\mu} = \frac{920 \times 300 / 60 \times (0.17)^2}{0.117} \left( \frac{kg/m^3 \times rev/s \times m^2}{kg/m.s} \right)$$

$$N_{Re} = 1136.2$$

The Reynolds number is >400 [84], for this Reynolds we are using flat blade turbine and baffle. From this relation we can find inside heat transfer coefficient as the following relation.

$$h_i = \frac{k_f}{D_T} \times 0.74 \times \left( \frac{\rho N D a^2}{\mu} \right)^{0.67} \left( \frac{c_p \mu}{k} \right)^{0.23} \left( \frac{\mu b}{\mu_w} \right)^{0.14} \quad (5.16)$$

Properties of fluid (jatropha oil) [86];

$$\rho_{oil} = 920 \text{ kg/m}^3$$

$$\mu_{oil} = 0.117 \text{ kg/m.s}$$

$$C_{p_{oil}} = 4.25 \text{ kJ/kg.K}$$

$$k_{oil} = 0.082 \text{ w/m.}^\circ\text{C}$$

$$N = 300 \text{ rpm}$$

$$D_A = 0.17 \text{ m}$$

$$T = 30^\circ\text{C}$$

$$h_i = \frac{0.082}{0.5} \times 0.74 \times (1136.2)^{0.67} (6064.02)^{0.23} \times 1^{0.14} \quad (5.17)$$

$$\left( \frac{\mu b}{\mu_w} \right) \cong 1$$

$$h_i = 50.14 \frac{w}{m^2.k}$$

b) Calculation of Fouling factors and wall resistances

Experience and judgment is required for the severity of fouling (**FF<sub>i</sub>**, **FF<sub>j</sub>**) to determine the heat transfer coefficient. This will depend on the efficiency and cleaning of the vessel.

c) Outside coefficient (**h<sub>o</sub>**) jacketed vessels

Annular jacket with no baffles

In the case of steam condensation, a film heat transfer coefficient **h<sub>j</sub>** is used. In case of fluid circulation, velocity will be very low because of the large cross-sectional area.

In tube flow the convection heat transfer coefficient is usually defined by;

Local heat flux,

$$q'' = h \times (T_w - T_b) \quad (5.18)$$

There are several areas that need to be calculated:

i. Heat transfer area of cylindrical part of reactor (i.e. jatropha oil and ethanol);

$$A = \pi DL = \pi \times 0.50 \times 0.75$$

$$A = 1.18m^2$$

ii. Heat transfer area of jacket for steam flow rate,

$$A = \pi DL$$

$$A = \pi \times 0.60 \times 0.68$$

$$A = 1.3m^2$$

iii. Heat transfer surface area of reactants,

$$A = \pi D_i L = \pi(0.50m) \times 0.95m = 1.5m^2$$

Note that the only outside surface of the inner tube transfer heat to the reactant. The overall annular dimensions, however, influence the hydraulic diameter which must be used to calculate the Reynolds number, and subsequently the heat transfer coefficient for the steam. The hydraulic diameter for the steam flowing in the annular section is calculated using the equation,

$$D_H = \frac{4A_c}{P} = d_{jo} - d_{io} = 0.610 - 0.510 = 0.1m$$

### 5.5. Energy balance in jacketed reactor

From the conservation of energy it can be written as:

$$\{\text{energy through system boundaries}\} - \{\text{energy out through system boundaries}\} = \{\text{energy accumulated within the system}\}$$

Mass  $m_i$  enters the system and  $m_o$  leaves. Both have energy associated with them in the form of internal, kinetic and potential energy: flow work also being done. Energy leaves the system as heat  $Q$ ; shaft work  $W_s$ , is performed on the system by the surrounding. Specific energy conservation multiplied by mass,

$$m_i(u + e_k + e_p + pv)_i - m_o(u + e_k + e_p + pv)_o - Q + W_s = \Delta E \quad (5.19)$$

Where,  $\Delta E$  is the accumulation of energy. This energy is equal to zero when the system is steady state. In batch operations, there is the occurrence of two typical situations:

- i. The design parameter is the operation time for heating or cooling, hence the surface area is unknown
- ii. The area heat exchanger is unknown and the operation time is unknown

Three energy balances can describe the heat transferred in the vessel [87].

- First heat added by heating steam:

$$\dot{Q} = \dot{m}_j \cdot C_{p,j} \cdot (T_{j,out} - T_{j,in}) \quad (5.20)$$

Where,  $\dot{m}_j$  is the mass flow rate in the jacket,  $T_{j, out}$  and  $T_{j, in}$ , the temperature into and out from the jacket, respectively.

- The transmission through the wall:

$$\dot{Q} = UA\Delta T_{lm} \quad (5.21)$$

Where,  $A$  is the total heat transfer area and  $\Delta T_{lm}$  the logarithmic mean temperature difference.

- The last balance is the heat added to product:

$$\dot{Q} = m_v C_{pv} \frac{dT}{dt} \quad (5.23)$$

Where,  $m_v$  is the mass of the liquid in the vessel and  $T$ , the temperature of the liquid in the vessel.

Combining these three equations give following ordinary differential equation:

$$\frac{dT}{dt} = \frac{\dot{m}_j C_{p,j}}{m_v C_{p,v}} (T_{v,out} - T_j + (T_{v,in} - T_j)e^y) \quad (5.24)$$

$$y = \frac{UA}{\dot{m}_j C_{p_j}}$$

### 5.7.1. Changing the product temperature –heating the product with steam

The amount of heat required to raise the temperature of the substance can be expressed as:

$$Q = M_s h_{fg} = M_b C_p \Delta T \quad (5.25)$$

In non- flow applications a fixed mass or a single batch of product is heated. In flow type applications or continuous flow the product or fluid is heated when it is flow over a heat transfer surface.

### 5.7.2. Batch heating or non-flow

In non- flow type applications the process fluid is kept as a single batch within a tank or vessel. A steam jacket or steam coil is heats the fluid from a low to high temperature. The mean rate of heat transfer for such applications can be expressed as[87]:

$$\dot{Q} = mC_p \frac{\Delta T}{t} \quad (5.26)$$

Where,

q = mean heat transfer (kW (kJ/s))

m= mass of the product (kg)

C<sub>p</sub> = specific heat of the product (kJ/kg.°C)

ΔT = change in temperature of the fluid (°C)

t = total time over which the heating process occurs (second)

A quantity of jatropha oil heated with a maximum designed pressure of 1.5 bars from a temperature of 30 to 80 °C is 75kg. The specific heat capacity of Jatropha oil is 4.73kJ/kg.°c.

$$Q = M_s h_{fg} = M_b C_p \Delta T$$

The amount of heat required to raise the temperature of jatropha oil in the jacketed reactor is calculated from equation (5.24),

$$Q = 75 \times 4.73 \times 10^3 \times (80 - 30) \times (kg \times kj / kg.^{\circ} C \times^{\circ} C)$$

$$Q = 17737.5kJ$$

Amount of heat released from burning of jatropha is calculated from the following relation:

$$Q = M_s \times (h_g - h_f)$$

$$Q = 367 \times (2667.6 - 125.74) \times \left( \frac{kg}{hr} \times \frac{kJ}{kg} \right)$$

$$Q = 259.16kW$$

The rate of heat required to heat 75kg of jatropha oil ( $C_p=4.73kJ/kg$ ) from 30 °C to 80 °C heating temperature of jatropha oil with steam produced from jatropha cake boiler for 500 sec can be calculated by equation (5.25):

$$q = mC_p \frac{dT}{t}$$

$$q = \frac{mC_p dT}{t}$$

$$q = \frac{75 \times 4.73 \times 10^3 \times (80 - 30) \times (kg \times j / kg \cdot ^\circ C \times ^\circ C)}{500s}$$

$$q = 35.48kW$$

The condensation convection coefficient of jacketed reactor is calculated from the following relation. This heat is transferred through the wall of batch reactor to the jatropha oil by convection system from 30 °C to 80°C.

From equation (5.18), steam condensation can be calculated as follows:

$$h_o = \frac{Q}{A_s (T_s - T_\infty)}$$

$$h_o = \frac{259.16kW}{1.5 \times (95 - 30)(m^2 \times k)}$$

$$h_o = 2658 \frac{W}{m^2 \cdot k}$$

Typical overall coefficients for jacketed stainless steel vessels would be 400w/m<sup>2</sup>.k [88].

## 5.6. Computational modeling of jacketed reactor

### 5.6.1. Geometry and mesh generation

CFD analyses have been carried out. The fluent release 17.2 is used for numerical simulation. The jacketed vessel was created by **CATIA** software, the preprocessing of the fluent module code. The appearance of the vessel with the agitator is shown below.

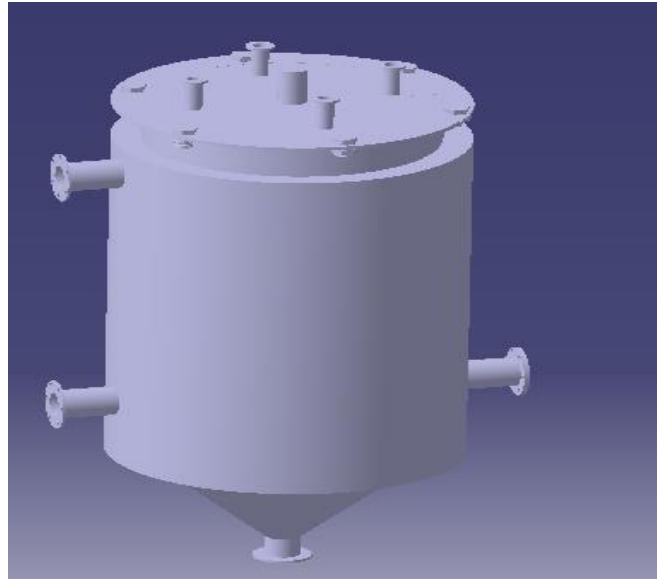


Figure 5.4: Stirred jacketed vessel assembly

The grid generation was formed by Grid. The geometry and the grid of jacketed vessel mesh are imported into fluent.

### 5.6.2. Model and Assumptions

Turbulent flow is a highly complex flow, where  $k-\varepsilon$  model has been validated many times. In this model, due to the complex structure inside the JHE,  $k-\varepsilon$  model is adopted for simulation in Fluent Release17.2. Here we simplify the model actual problem with the following assumptions: fluid flow inside is steady state turbulence; the fluid inside is Newtonian fluid; the density of fluid is regarded as a constant with no sharply change of temperature; the fluid satisfies the no-slip wall condition.

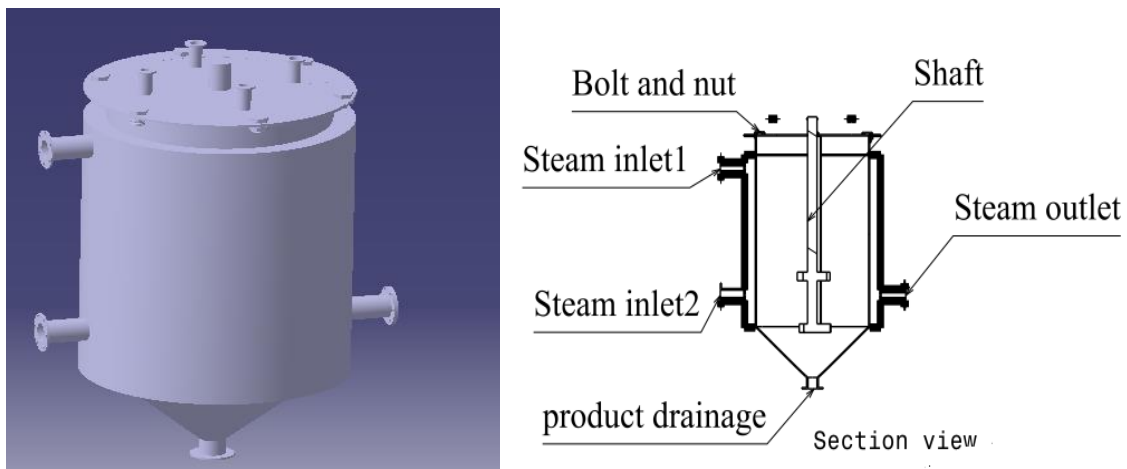


Figure 5.5 overall part names of the reactor with 3D drawing of jacketed reactor

As shown in Figure 5.5, the inside diameter of reactor is 500mm; outside diameter is 510mm; and the cylindrical height is 750mm. The jacket inside diameter is 600mm, outside diameter 610, and the height is 680mm. From the literature, the most applicable physics model is chosen to represent the different regions of the CFD simulation. The CFD model was modeled as an implicit and unsteady as this behavior is inherent to the condensation model in fluent software. The fuel /ethanol were modeled as volume of fluid as single phase. Steam is used for heating of the oil/ethanol during chemical reaction. An implicit coupling of thermal and hydrodynamic effects was enabled to model heating of the chemical reaction from 30-80°C to reduce the retention time and viscosity of the jatropha oil. Due to the turbulent nature of both steam and fuel, the realizable K-ε model was used to represent the physics.

### 5.6.3. Control Equations

From Navier-stokes equation, energy equation and momentum equation, we can solve the problem of turbulent flow.

The governing equations in Cartesian coordinate of turbulent flow can be written as follows:

$$\frac{\partial(\rho u)}{\partial t} + \text{div}(\rho u u) = \text{div}(\mu \text{grad} u) - \frac{\partial p}{\partial x} + F_x \quad (5.27)$$

$$\frac{\partial(\rho v)}{\partial t} + \text{div}(\rho v v) = \text{div}(\mu \text{grad} v) - \frac{\partial p}{\partial y} + F_y \quad (5.28)$$

$$\frac{\partial(\rho w)}{\partial t} + \text{div}(\rho w w) = \text{div}(\mu \text{grad} w) - \frac{\partial p}{\partial z} + F_z \quad (5.29)$$

K-ε Turbulence model

Where, k turbulent kinetic energy and it is the measure of how much energy is contained in the fluctuations.

ε: turbulent dissipation and the measure of the rate at which turbulent kinetic energy dissipated.

Unknown turbulent terms are calculated from k and ε.

$$\rho(\vec{V} \cdot \nabla) \vec{V} = -\nabla p + \mu \nabla \cdot (\nabla \vec{V} + \nabla \vec{V}^T) - \frac{2}{3} \mu \nabla (\nabla \cdot \vec{V}) \quad (5.30)$$

#### 1. Boundary Conditions

Here, we set the fluid in jacketed heat exchanger is the steam temperature 368K, the outface set as pressure outlet. The temperature of inside fluid is 303K, and the out face is set as no heat transfer to the atmosphere

## 2.Reynolds averaged three governing equation with k-ε Model

### a.Conservation of mass

$$\nabla V \cdot (\rho \vec{V}) = 0 \quad (5.31)$$

### b. Conservation of momentum (F=ma in axial and radial directions)

$$\rho(\vec{V} \cdot \nabla) \vec{V} = -\nabla p + \mu \nabla \cdot (\nabla \vec{V} + \nabla \vec{V}^T) - \frac{2}{3} \mu \nabla (\nabla \cdot \vec{V}) \quad (5.32)$$

### c.Conservation of energy (first law of thermodynamics)

$$\rho(\vec{V} \cdot \nabla)(CvT) = k \nabla^2 T - p(\nabla \cdot V) + \mu \phi + \text{turbulent terms} \quad (5.33)$$

Where, + Turbulent terms

### d. Ideal gas law

$$\rho = \frac{P}{RT} = \frac{P_{average}}{RT} \quad (5.34)$$

### e.K conservation equation

### f. ε conservation equation

✓ 7 unknown functions: Vr, Vz, P, T, ρ, k, ε

## CHAPTER SIX 6

### RESULTS AND DISCUSSION

The steam side geometry and reactor was simulated for the purpose of this study. The input heat parameters of the study were taken from steam boiler and the material properties of the variables. The outside temperature of the feed steam is assumed as constant temperature boundary. The feeding of reactants is assumed unsteady and the heat is transferred through system coupling of the jacket wall and the reactor wall through convection and conduction process. Initially the temperature of the steam required was designed at minimum temperature of water boiling point  $95^{\circ}\text{C}$  for both inlets at 1.5bar pressure. The batch reactants feed at room temperature and pressure. After time duration the temperature of the reactant arrived the maximum reaction temperature of  $80^{\circ}\text{C}$ . The main purpose of this study was to analysis the heat transfer system and thermal properties of reacting materials. A jacketed vessel is used for the production of biodiesel with the mixing of Jatropha oil and ethanol fuel. For this study, we are concerned on the simulation of heat transfer between the jacket and vessel with the kinetics of reaction. The hot steam flow is jetted into the jacket through two nozzles after the Jatropha oil/ethanol is added through two nozzles through the top of the vessel.

#### 6.1. Numerical simulation

Steam is used as heating medium in jacketed vessel.

The simulation of the jacketed vessel is performed with the following assumptions:

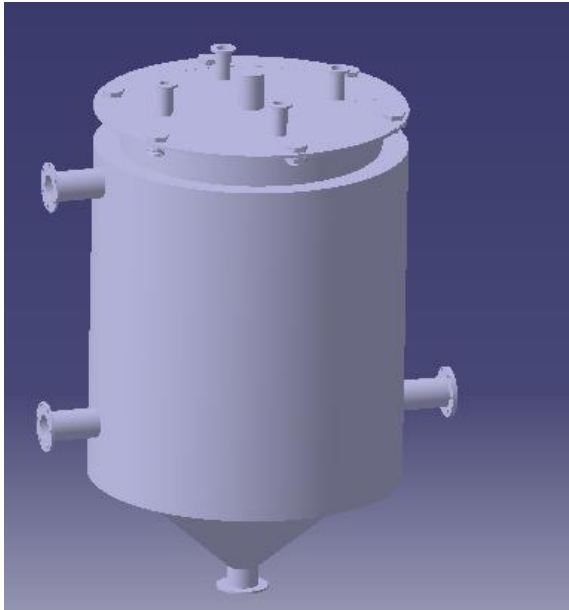
- No phase change takes place in the jacketed vessel
- There is no heat loss in the jacketed vessel to the environment
- The steam flow is steady and incompressible
- The material properties of the materials are constant

The continuity principle is used to couple the simulation process of the jacket and vessel. The temperature and heat flux released by the heat transfer surface of the jacket and vessel is the same. This chapter discusses the result obtained from the simulation runs for the heat transfer analysis in the jacketed reactor.

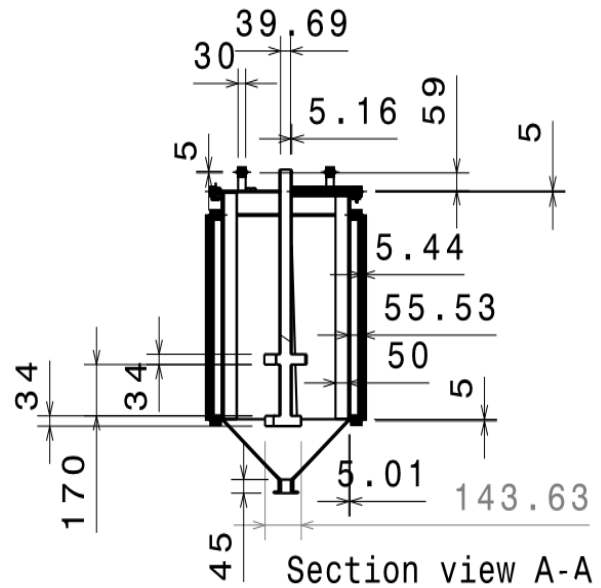
The simulation is performed by three steps:

### i. Geometry modeling

The geometry modeling is represented jacketed batch reactor. Three models with different inlet of the geometry were created for the purpose of CFD analysis. All models were created by CATIA software V5R19. These files were imported into Ansys release 17.2 fluent for CFD analysis.



(a)



(b)

Figure 6.1 (a) represents jacketed agitator vessel (b) jacketed vessel section view of the model

The 3D CATIA included 750mm cylindrical reactor with 100mm conical reactor and 680mm jacket on the outside of the reactor. It is important to make adiabatic heat transfer from the surface of the jacket due to covering the system by insulation. The Jatropa oil and ethanol is modeled on the inside of steel reactor. Steam is flowing into the jacketed reactor through two inlets to avoid heat spots at one location during flowing and has one outlet.

### ii. Meshing /discretizing of the geometry

Meshing is an integral part of a CFD simulation. It is important to correctly have optimum number of cells to analysis the physical interaction taking place in the simulation. During this time the boundary of simulation assigned and the number of cell zones is done.

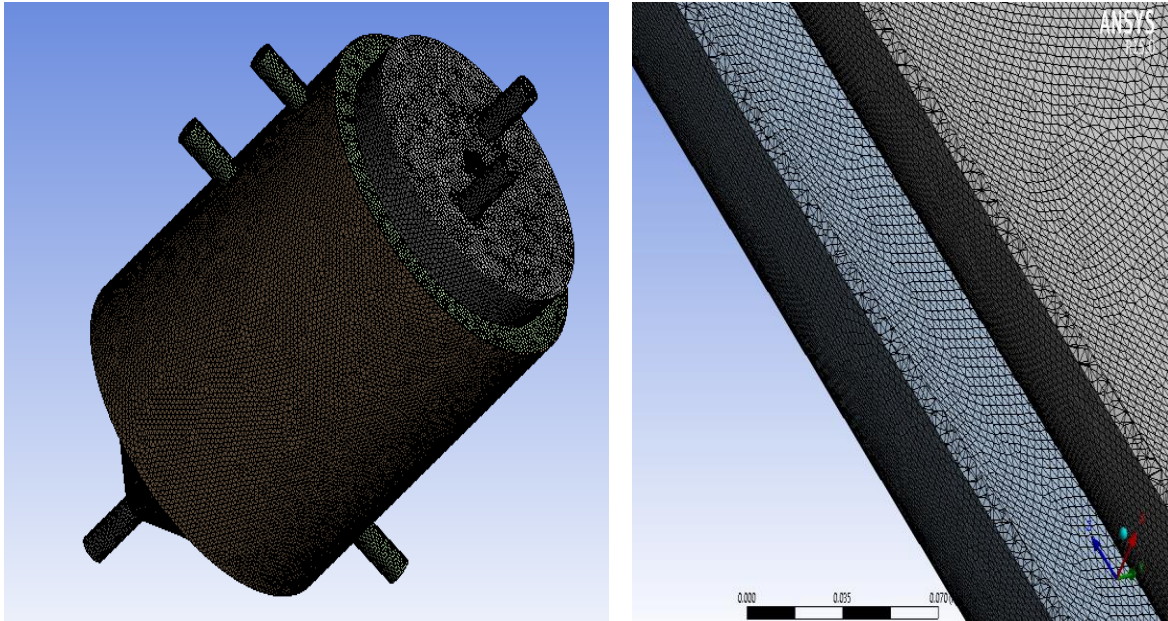


Figure 6.2 Meshing of the assembled vessel system discretized at different elements

Details of "Mesh"	
<input checked="" type="checkbox"/> Assembly Meshing	
<input checked="" type="checkbox"/> Advanced	
<input checked="" type="checkbox"/> Statistics	
<input type="checkbox"/> Nodes	207143
<input type="checkbox"/> Elements	924182
Mesh Metric	
<input type="checkbox"/> Min	2.357e-007
<input type="checkbox"/> Max	0.97923
<input type="checkbox"/> Average	0.24462
<input type="checkbox"/> Standard Deviation	0.12648

From this mesh, the quality of skew mesh is less than 0.98 to converge the solution of fluent simulation. At this mesh quality, the simulation is converged.

### iii. Post processing /Fluent simulation

The simulation is run under coupled method instead of single method. This means the heat transfer modeling of the jacket and vessel/reactor done together instead of separate simulation. The result converges after flow time of 500s and 1 time steps.

The time dependence of temperature on the batch reactor and process side heat transfer coefficient were evaluated for the wall surface and the bottom conical surface while heating with constant temperature of 95°C heating medium temperature. The functional relationship between the nusselt and reynolds number was correlated to determine the process side heat transfer coefficient of the heat transfer wall. The reference temperature of the batch was

30°C as initial temperature of the batch. From the simulation result, the turbulence of energy is high at the outlet of the jacket. From the inlet of the jacket, little bit amount of spot is formed but uniform heat transfer is happen on the wall of the vessel.

### 6.1.1. Simulation result of stirred reactor system

This simulation result indicates the mixing of batch reactant in the stirred reactor by using agitator. The reactor is assembled with baffling system to make homogeneous mixing of chemical reactant. The stirring purpose is mainly done by using two impellers far apart 170mm. This system consumes power for the running of impeller by motor system. As we can see from simulation result, the temperature contours are high at the wall of batch reactor. For facilitating of mixing, flat blade turbine is used to reduce the viscosity of jatropha oil under the chemical reaction.

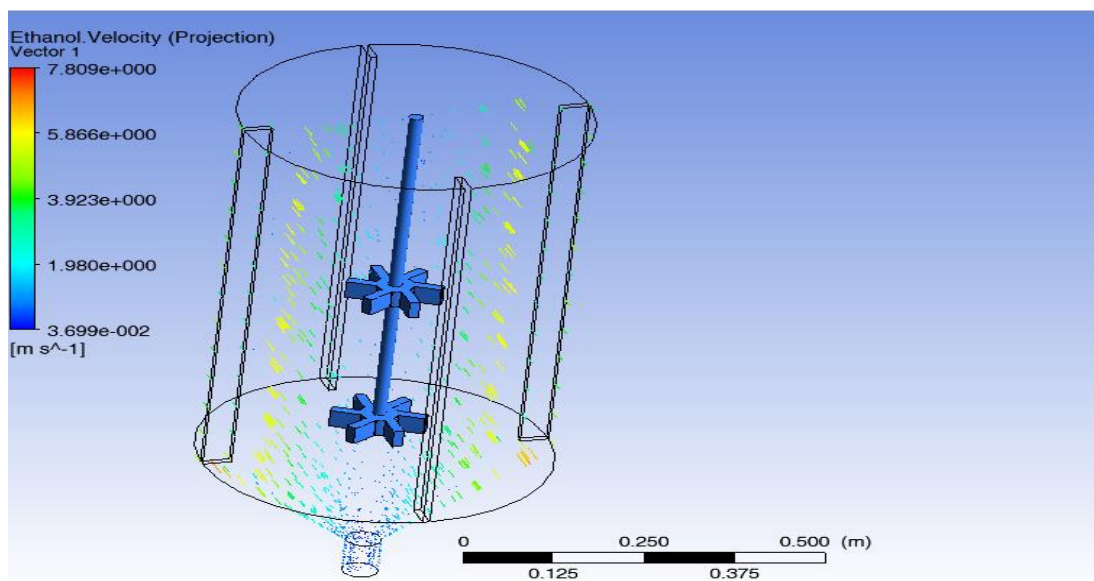
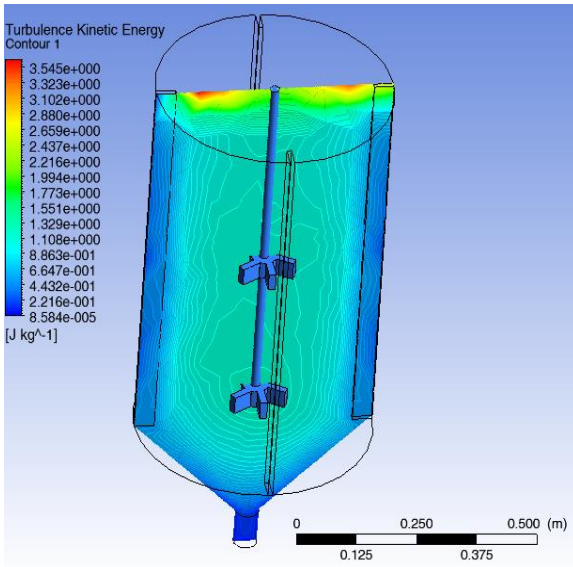
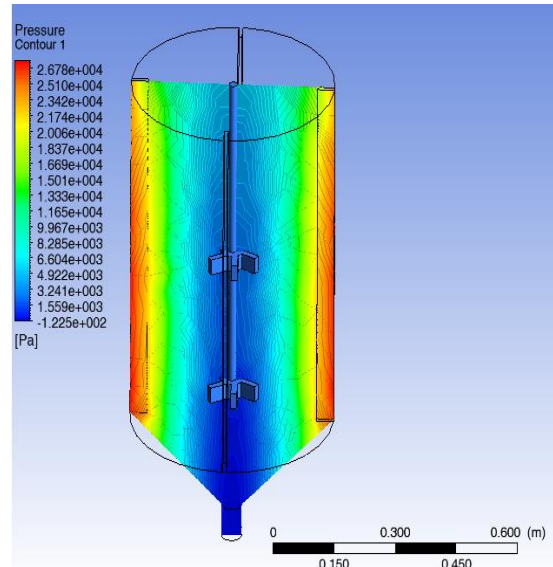


Figure 6.3 velocity vector of the incoming batch fuel in the chemical reactor

The fluid flow in the batch reactor is uniform along the cross-section. This means the speed of mixing by agitator system by using two impellers far apart at 170mm. As the number of impeller is increased, uniform mixing of fluid is happened.



(a)



(b)

Figure 6.4 (a) and (b) shows the plane section of turbulence kinetic energy contour and pressure contour in stirred reactor during chemical reaction respectively.

The above figure shows, turbulent kinetic energy is high at the inlet of the batch reactor and the pressure distribution is high at the wall of batch reactor. This is due to the internal pressure coming from stirring and external pressure which is applied from steam energy through inlet nozzle. The outlet turbulence of the baffled reactor and pressure is reduced. At outlet the pressure is reduced to the atmospheric pressure.

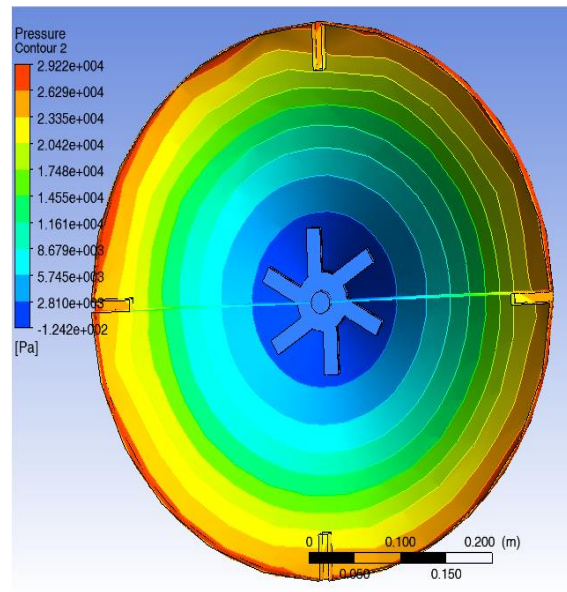
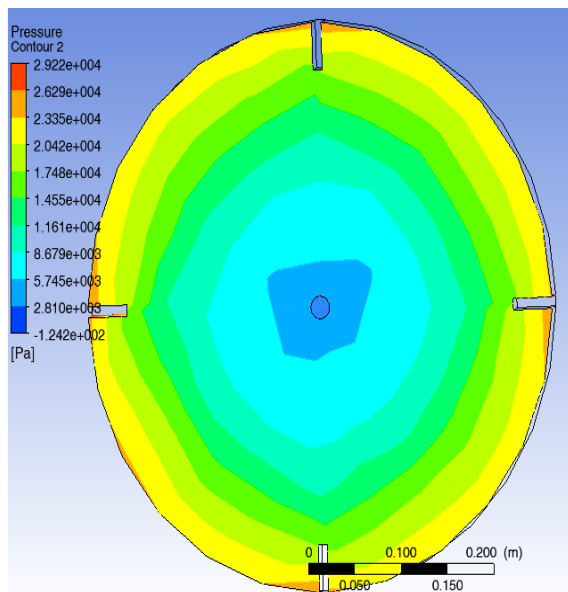


Figure 6.5 the stirring or mixing of fuel system with the ethanol with baffled reactor

From the above simulation, the fluid flow during mixing is uniform through the cross-section of reactor. Vortex formation is avoided by using baffle and flat blade turbine at 300rpm of impeller system. Stirring system is used for mixing of one phase liquid to speed up the chemical reaction.

### 6.2.1. Jacketed vessel simulation result

The jacketed reactors have different temperature distribution due to the heating energy of steam energy through the annular cross section of the reactant. The main purpose of jacketing heat transfer is to raise the temperature of batch reactant from 30 to 80 degree Celsius. This temperature is the maximum temperature of batch reactant during chemical reaction to reduce the retention time of the chemical reaction. This reactor can hold 0.15m<sup>3</sup> of reactant with flat cover with conical bottom to facilitate the settling of the product while draining of the by product.

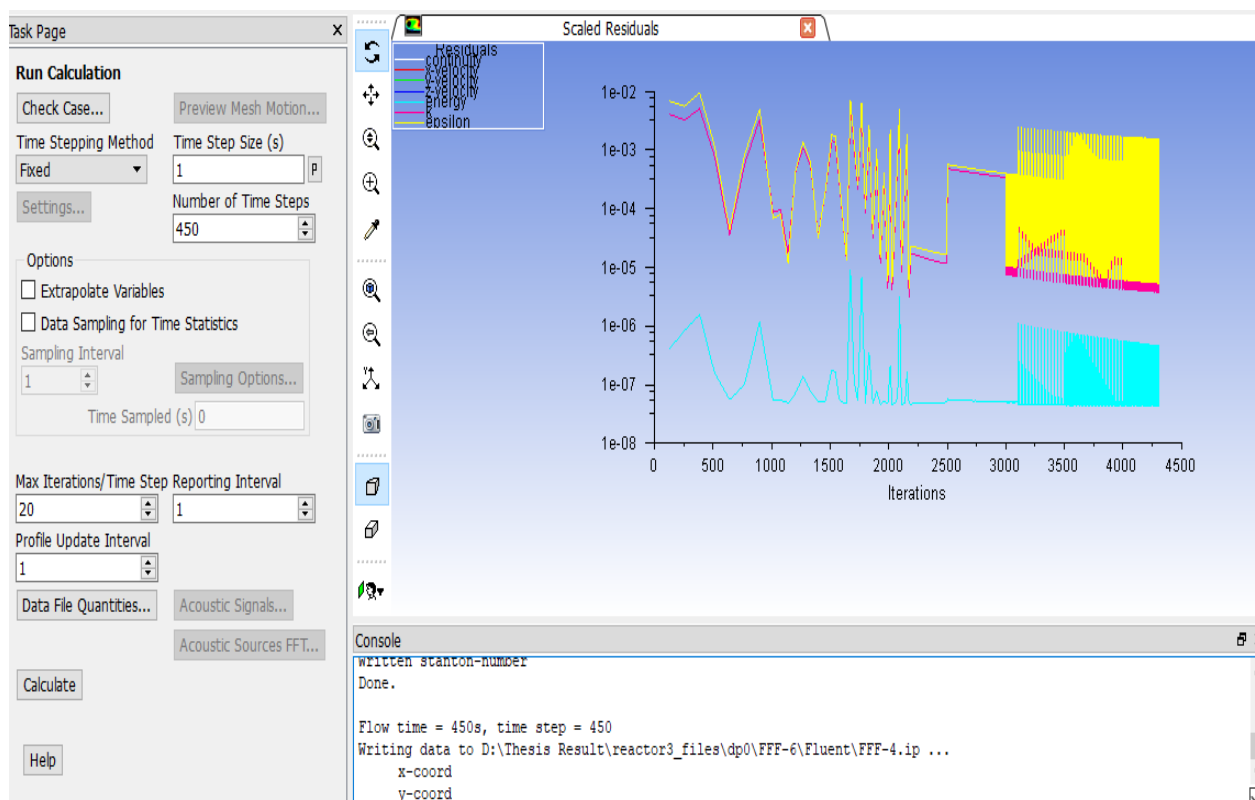
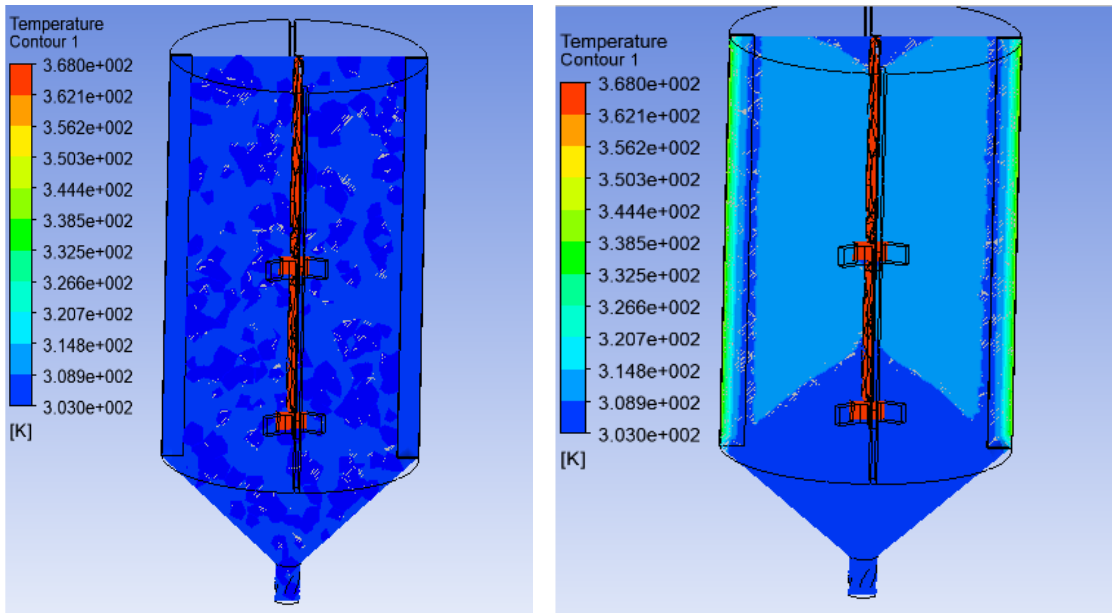


Figure6.6. Solution iteration of transient fluid flow convergence diagram

The following figures show the Temperature contours during transient simulation within 500s duration of heating in the batch reactors. At the initial time of simulation, temperature contour is uniform in the process fluid. That means before the start of heat transfer from

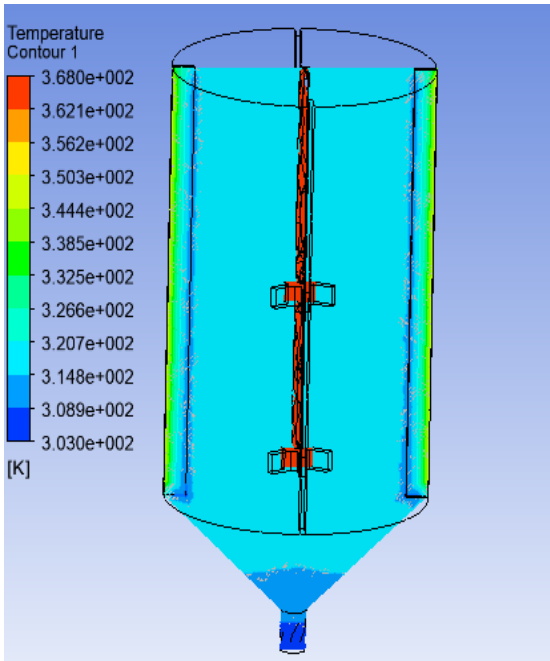
steam system to the batch reactor, the process fluid temperature is 30°C. From this duration to 500s, the temperature contour is different from the reactor surface to the process fluid.



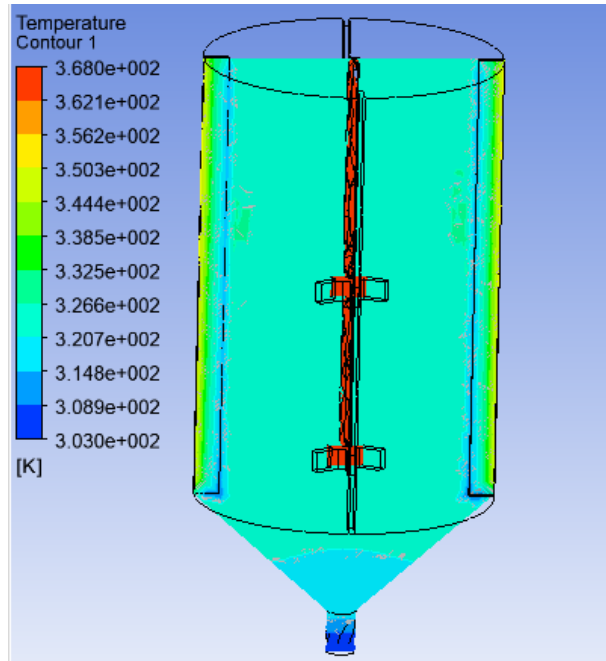
(a) at 0s

(b) at 1s

As we can see from figure (a) simulation time, the temperature of the system was 30°C throughout the reactant for the initial time. But for the 1<sup>st</sup> heating time, the temperature of the process fluid started to be increased from 303K to 314.8K. As the time increased, the heat transfer increased from the wall of reactant to the process fluid. This heat energy was generated from external steam energy which was generated from Jatropa cake boiler after the burning of jatropa cake. The temperature of the steam system was assumed 368K; this amount of steam temperature was transferred by convection heat transfer to the process fluid. The amount of convection coefficient transferred through the wall of jacketed vessel steel was 2658w/m<sup>2</sup>.K at the value of this steam temperature.

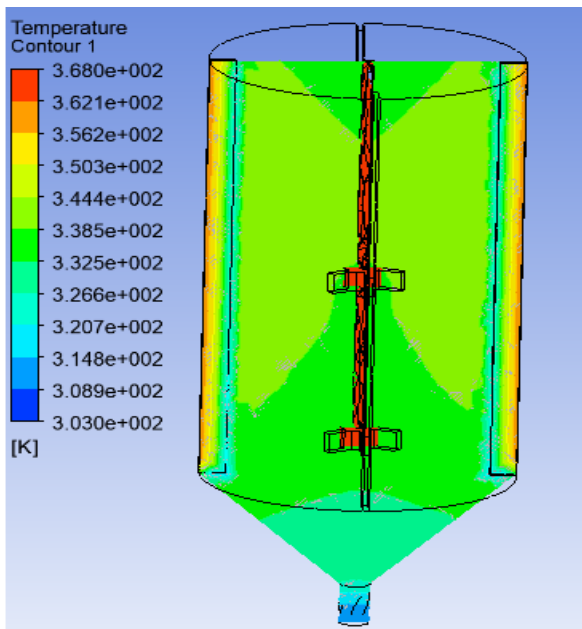


(c) at 3s

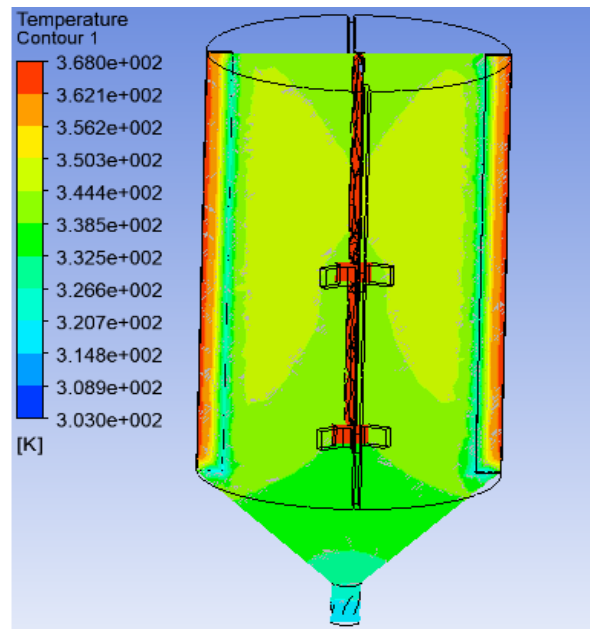


(d) at 5s

At 3s of simulation time, the temperature of process fluid is increased to 320.7k from the above figure (c) and it also increased to 326K as seen from figure (d) at 5s. The boundary of the system was 368K temperature and  $2658\text{w/m}^2\cdot\text{K}$  convection coefficient through the wall of the reactor.

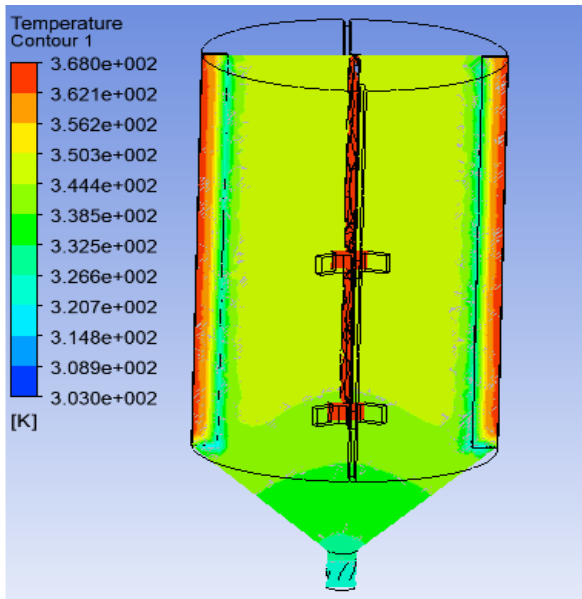


(e) at 20s

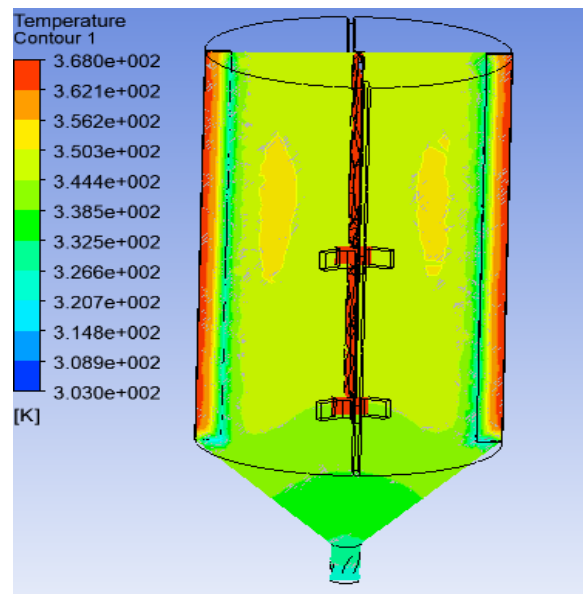


(f) at 60s

After 20 to 60s simulation time, the temperature of process fluid is increased to around 332K to 344K as we can see from the above figure of temperature contour.

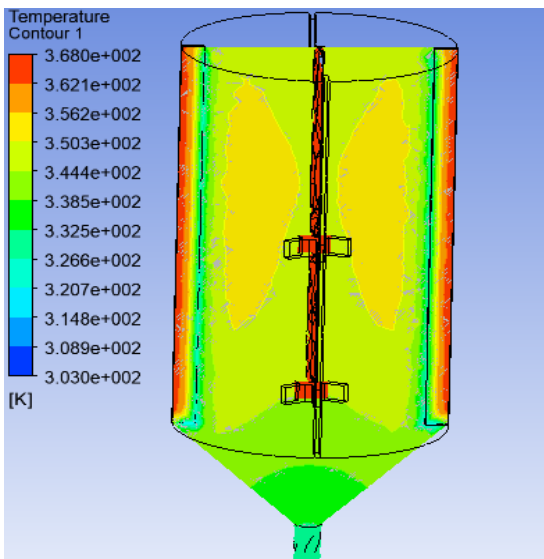


(g) at 120s

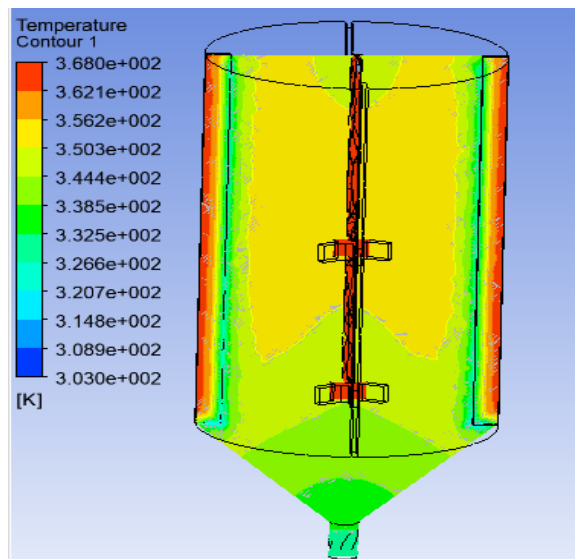


(h) 160s

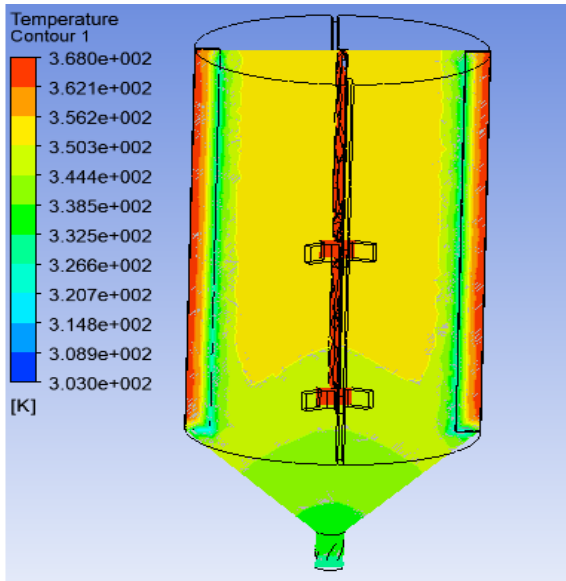
From figure (g) and (h) temperature contour from 120s to 160s simulation time, the temperature of the process fluid is partially increased to 347K.



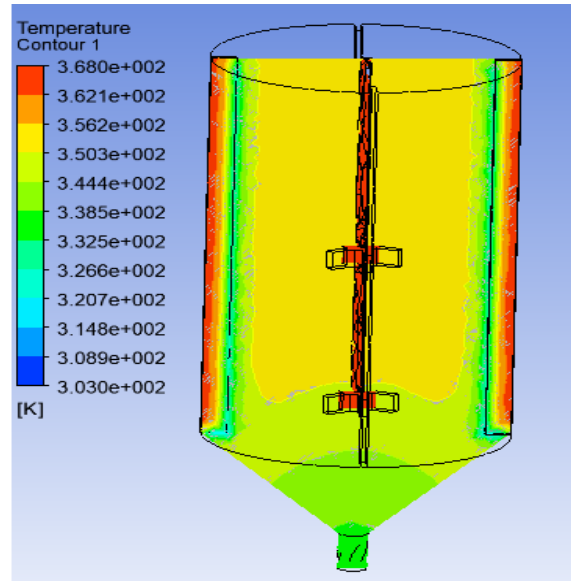
(i) At 200s



(j) at 250s

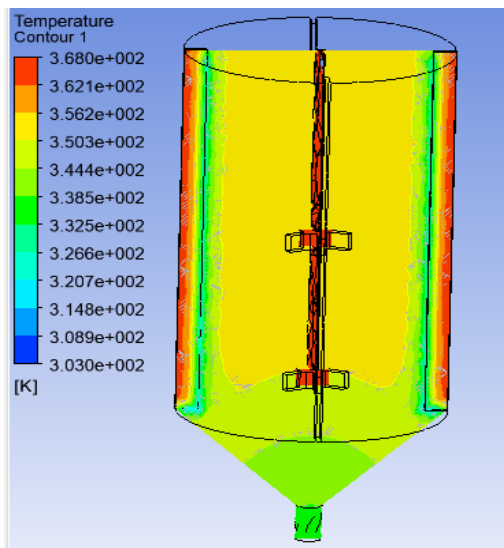


(k) at 300s

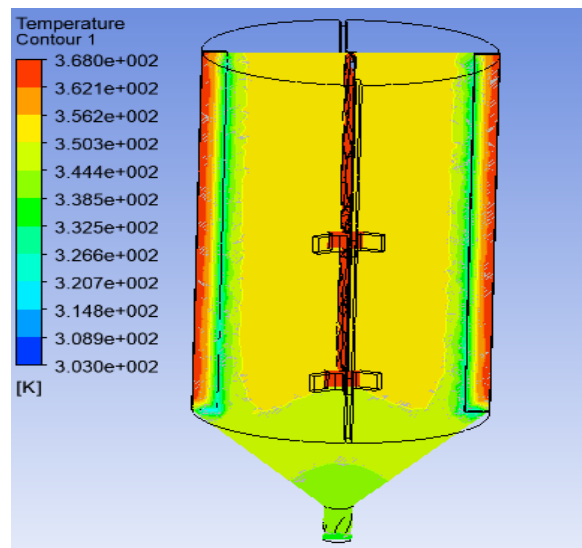


(l) at 360s

Generally, the simulation result indicates the temperature of process fluid is increased to 353K from 303K at 500s. The cylindrical part of the reactor is jacketed and the cover head and bottom conical reactor is insulated to prevent heat loss from the system.



(m) at 400s



(n) at 500s

Figure 6.7 from a-n shows temperature distribution during heating of batch reactor at different times

The temperature of heating steam is 368K on the wall of jacketed reactor. The heat transfer of stainless steel wall is very good and the heat loss is low due to the insulating material coating on the jacketed reactor. No heat loss is happened at the conical shape of the reactor

and heat is transferred from the wall of the reactor to the batch fluid to raise the temperature of the batch fluid from 303 to 353K for 500s heating process by using 412.16KJ capacity of jatropa cake boiler. From this capacity of boiler, 269.81KJ heat energy is transferred by convection and conduction heat transfer system to heat 75kg of batch reactant in the reactor. This heat transfer is required during speed up of reacting jatropa oil with the mixture of ethanol alcohol. This temperature is the maximum limiting value of biodiesel synthesis by transesterification reaction.

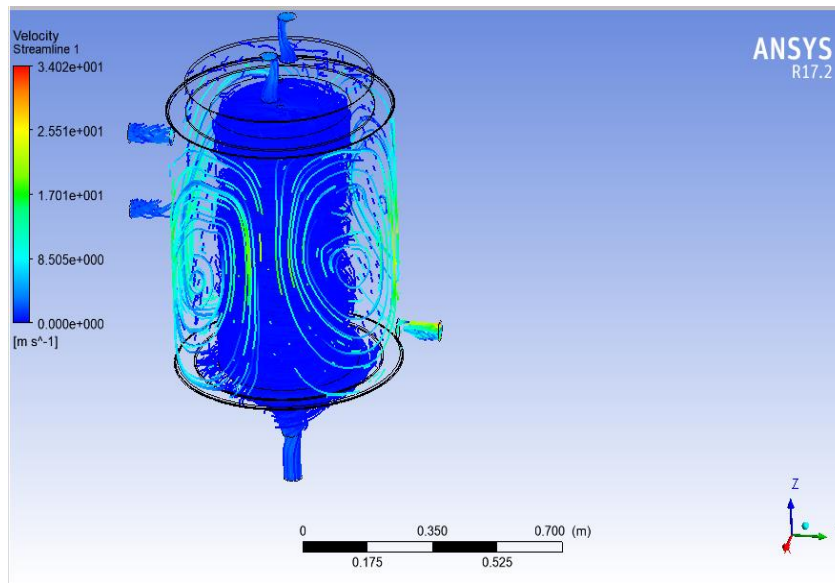


Figure 6.8 stream line flow of incoming fuel in the batch reactor

From this stream line, we can visualize the speed of steam coming in through the jacket inlet and reactor inlet. The steam is distributed through the annular section of the jacketed reactor uniformly due to two inlet mass flow rate of steam. The velocity of incoming fluid is greater than the batch reactant due to the density of the fluid flowing in. The fuel coming in is swirled by impeller and the stream line is somewhat uniform at low speed of agitation system. The maximum oil velocity is 1.2 m/s batch reactor and 2-3m/s velocity of steam coming in through the jacket inlet. But, most part of fuel velocity is around 0-34.2 m/s. Therefore the calculated incoming fluid velocity is in the range of the simulated values.

This result shows that trans-esterification reaction was depending on the rate of temperature difference. The maximum temperature of reaction is depends on the boiling point of alcohol. The alcohol used was ethanol which has 80 °C boiling points. At the maximum of 80 °C, the retention time or the rate of reaction was reduced to 8 minute from 20 minute as seen from Tint et.al, (2009). Some groups use a two-step reaction, with glycerol removal between

steps, to increase the final reaction extent to 95%. Higher temperatures and higher alcohol: oil ratios also can enhance the percent completion. Typical reaction times ranges from 20 minutes to more than one hour[54]. This variation of result was come from constant heating and adequate mixing of ethanol and Jatropha oil at 300rpm stirring by six flat blade turbine. The main purpose of the thesis was to reduce the retention time of chemical reaction by designing of an external jacketed reactor. The analysis refers to the heating process of the fluid. The temperature of vegetable was increased due to thermal energy provided by Jatropha cake boiler. In particular, the transient temperature effect was studied together with the flow field within the batch reactor, once an initial vegetable oil temperature of 30°C and a final temperature of 80°C have been chosen. The higher reaction temperatures exhibit the rate of the trans-esterification reaction and the FAEE yield. Temperature effects are reported to be pronounced for the rates of transesterification reaction[89-90]. Of interest is also the temperature dependence of the maximum FAEE yields. The yield was highest at 70°C (98%), and reduced to 93 and 91 % for reactions at 50 and 30 °C respectively[90]. These data suggest that the equilibrium position of the transesterification reaction shifts to the right at higher temperatures, implying that the trans-esterification reaction is slightly endothermic. Similar temperature dependencies of the equilibrium position were observed by Narvaez et al. [91] for palm oil methanolysis. Here, the maximum (equilibrium) conversion increased from 90.6% at 50°C to 90.3% at 60°C. Nouredini and Zhu[92] reported that the maximum conversion for the transesterification of soybean oil at 70°C (90%) is considerably higher than at 50°C (80%). In addition, Vicente et al. [91] reported that the maximum conversion at 65°C (99%) is higher than at 25°C (94%) for sunflower oil methanolysis.

## CHAPTER 7

### CONCLUSION AND RECOMMENDATION

Biodiesel is a renewable source of fuel energy and can be used in engine with or without blending of diesel fuel. Biofuel energy which is generated from Jatropha oil is viscous and has high purification property. Hence, to solve such problem blending of the fuel by B100:100, B10:100, B20:100 of the petrol fuel. Biodiesel is produced from Jatropha oil by transesterification with ethanol mixing in the presence of NaOH or KOH in the batch reactor. The chemical reaction takes place within different parameters such as temperature, pressure, and ethanol: oil molar ratio, catalyst concentration and retention time. Heat is transferred to or from a system. To add heat energy to the system, heat energy is added to increase the internal energy of the system. The transfer of heat takes place without the contact of fluid system. This means, hot and cold fluid does not mix each other during heat transfer process. This method is called as indirect heat transfer process. The heat transfer area is applied to the reactor by making jacketed reactor on the surface of the chemical reactor. This heating process is used to reduce the retention time of chemical reaction and speed up of the reaction to yield efficient product from the chemical reaction. Therefore, appropriate reactor is designed for the production of biodiesel in different reactor. Due to its simplicity and availability, the batch reactor is used from simple to medium size. This reactor is integrated with baffle, agitator, nozzles and jackets to facilitate the chemical reaction and heat transfer process. The reactor size is designed and modeled by mathematical method and the simulation of heat transfer process is done by fluent release 17.2. The simulation of the system is done by finite volume method and the size of the reactor discretized into different meshing. After it is discretized into appropriate mesh and importing into fluent solution method. After this method is progressed, the result of the heat and pressure distribution is done. The temperature of heating steam is fixed to around 368K and the reaction system is done at 353K. In the heating of 75kg of batch reactant, 269.81kJ energy is transferred for 500s. This heating value is generated from 412.16kW of jatropha cake boiler by burning 75kg of jatropha cake. Generally, heat energy is transferred to the reactor system through integration of nozzle inlets and outlets on the jacket of the reactor. From this study we conclude that the heat transfer system in jacketed vessel is affected in the interface boundary and the mass flow rate of the reacting fuel oil.

## **RECOMMENDATION**

- Designing of spiral jackets for the batch reactor to distribute heat energy uniformly
- Validation of the CFD simulation by experimental method and geometry modeling.
- Selecting of appropriate heat transfer area for the reactor and design of safe storage tanks for the system.
- Transesterification effects on the fluid domain properties will be analyzed in further works.
- Design of integrated steam boiler and economizer to reduce the loss of energy and to produce continuous amount of products
- Make durable and feasible system design for the appropriate results and environmental feasible project.
- Develop automatic control of steam supplied to the reactor with digital control system and safety devices during the chemical reaction
- Manufacturing of the reactor integrated with steam boiler and agitator in the system of the plant in addition to jacketing the reactor
- The sizing of the fire tube boiler is don't done in this thesis due to the bulky of the works I have done during the design of reactor.
- Trans-esterification effects on the fluid domain properties will be analyzed in further works.

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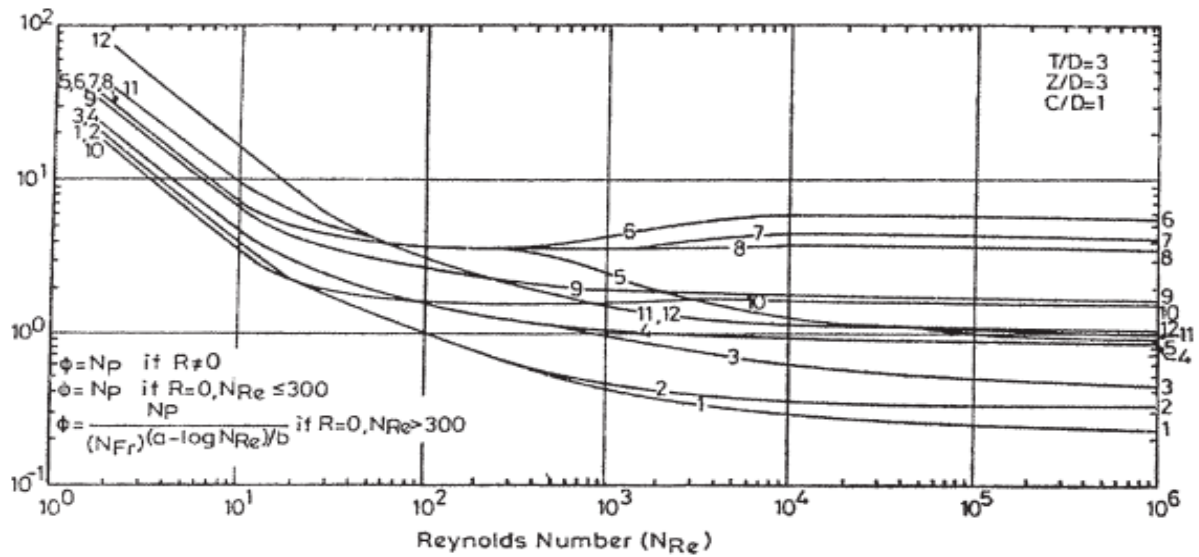
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## APPENDIX

### A. Power number correlation for different impeller



- |   |  |
|---|--|
| <p>1. Propellers, <math>\rho = D</math>; <math>R = 0</math><br/> <math>a = 2.1</math>, <math>b = 18</math>, <math>B = 3</math></p> <p>2. Propellers, <math>\rho = D</math>; <math>R = 4</math><br/> <math>J = 0.1 T</math>; <math>B = 3</math></p> <p>3. Propellers, <math>\rho = 2D</math>; <math>R = 0</math><br/> <math>a = 1.7</math>; <math>b = 18</math>; <math>B = 3</math></p> <p>4. Propellers, <math>\rho = 2D</math>; <math>R = 4</math><br/> <math>J = 0.1 T</math>; <math>B = 3</math></p> <p>5. Flat blade disc turbine,<br/> <math>R = 0</math>; <math>a = 1</math>; <math>0</math>; <math>b = 40.00</math></p> <p>6. Flat blade disc turbine,<br/> <math>R = 4</math>; <math>J = 0.1 T</math>; <math>B = 6</math></p> | <p>7. Curved blade disc turbine,<br/> <math>R = 4</math>; <math>J = 0.1 T</math>; <math>B = 6</math></p> <p>8. Arrow-head disc turbine,<br/> <math>R = 4</math>; <math>J = 0.1 T</math>; <math>B = 6</math></p> <p>9. Pitched blade turbine,<br/> <math>R = 4</math>; <math>J = 0.1 T</math>; <math>B = 8</math></p> <p>10. Flat paddle,<br/> <math>R = 4</math>; <math>J = 0.1 T</math>; <math>B = 2</math></p> <p>11. Shrouded turbine,<br/> <math>R = 4</math>; <math>J = 0.1 T</math>; <math>B = 6</math></p> <p>12. Diffuser ring shrouded turbines<br/>           stator ring having 20 blades,<br/> <math>B = 6</math>.</p> |
|---|--|

Power number versus Reynolds number correlation for common impellers. (Source: Rushton et al., [60].)

## Appendix B-Equations for calculating film coefficients of jacketed agitated vessels

**Table B-1**  
Equations for calculating inside film coefficients ( $h_i$ ) of jacketed agitated vessels

Agitator type	Baffled?	Reynolds number ( $N_{RE}$ )	Nusselt number ( $N_{Nu}$ )	Remarks
Paddle	Yes/No	$20 < N_{RE} < 4,000$	$0.415 (N_{RE})^{0.67} (N_{Pr})^{0.33} (\mu_b/\mu_w)^{0.14}$	Vessel geometry is discussed by Holland and Chapman [4]
Paddle	Yes/No	$>4,000$	$0.36 (N_{RE})^{0.67} (N_{Pr})^{0.33} (\mu_b/\mu_w)^{0.14}$	Vessel geometry is discussed by Holland and Chapman [4]
Flat blade turbine	Yes/No	$<400$	$0.54 (N_{RE})^{0.67} (N_{Pr})^{0.33} (\mu_b/\mu_w)^{0.14}$	$D_A/D_T = 1/3$ , $H/D_T = 1.0$ . Six-bladed turbine. Standard geometry.
Flat blade turbine	Yes	$>400$	$0.74 (N_{RE})^{0.67} (N_{Pr})^{0.33} (\mu_b/\mu_w)^{0.14}$	$D_A/D_T = 1/3$ , $H/D_T = 1.0$ . Six-bladed turbine. Standard geometry.
Flat blade turbine	Yes	$2,000 < N_{RE} < 700,000$	$1.10 (N_{RE})^{0.62} (N_{Pr})^{0.33} (\mu_b/\mu_w)^{0.14}$	
Propeller	Yes	$>5,000$	$0.64 (N_{RE})^{0.67} (N_{Pr})^{0.33} (\mu_b/\mu_w)^{0.14}$	Three blades
Propeller	Yes	No limitation	$0.54 (N_{RE})^{0.67} (N_{Pr})^{0.25} (\mu_b/\mu_w)^{0.14}$	45° pitched, four-blade impeller. Equation is based on limited data with regard to propeller pitch and vessel baffling. Divide $h_i$ obtained with this equation by a factor of about 1.3.
Retreating blade turbine	Yes	No limitation	$0.33 (N_{RE})^{0.67} (N_{Pr})^{0.33} (\mu_b/\mu_w)^{0.14}$	Glassed-steel impeller. Three retreating blades. The lower constant (0.33) for the glassed-steel impeller is attributed to greater slippage around its curved surfaces than around the sharp corners of
Retreating blade turbine	Yes	No limitation	$0.37 (N_{RE})^{0.67} (N_{Pr})^{0.33} (\mu_b/\mu_w)^{0.14}$	Alloy-steel impeller. Three retreating blades.
Retreating blade turbine	No	No limitation	$0.68 (N_{RE})^{0.67} (N_{Pr})^{0.33} (\mu_b/\mu_w)^{0.14}$	Six retreating blades.
Propeller	Yes	No limitation	$0.54 (N_{RE})^{0.67} (N_{Pr})^{0.25} (\mu_b/\mu_w)^{0.14}$	45° pitched four bladed impeller. Equation is based on limited data with regard to propeller pitch and vessel baffling. Divide $h_i$ obtained with this equation by a factor of about 1.3.
Anchor	No	$30 < N_{RE} < 300$	$1.0 (N_{RE})^{0.67} (N_{Pr})^{0.33} (\mu_b/\mu_w)^{0.18}$	The overall heat transfer coefficient $U$ , varies inversely with the anchor to-wall clearance. Anchor to wall clearance is less than 1 in.
Anchor	No	$300 < N_{RE} < 4,000$	$0.38 (N_{RE})^{0.67} (N_{Pr})^{0.33} (\mu_b/\mu_w)^{0.18}$	Similar condition as before.
Anchor	No	$4,000 < N_{RE} < 37,000$	$0.55 (N_{RE})^{0.67} (N_{Pr})^{0.25} (\mu_b/\mu_w)^{0.14}$	Anchor to wall clearance of 1 to 5.125 in. Vessel geometry is illustrated by Holland and Chapman [4]
Helical ribbon	No	$<130$	$0.248 (N_{RE})^{0.5} (N_{Pr})^{0.33} (\mu_b/\mu_w)^{0.14} \times (e/D_A)^{-0.22} (i/D)^{-0.28}$	$e$ = clearance, $(D_T - D_A)/2$ , ft $D_A$ = impeller diameter, ft $i$ = agitator-ribbon pitch, ft
Helical ribbon	No	$>130$	$0.248 (N_{RE})^{0.67} (N_{Pr})^{0.33} (\mu_b/\mu_w)^{0.14} \times (i/D)^{-0.25}$	Same as above.

**Table-B2**  
Equations for calculating outside film coefficients ( $h_o$ ) of jacketed agitated vessels

Jacket type	Reynolds number ( $N_{Re}$ )	Nusselt number ( $N_{Nu}$ )	Remarks
Annular jacket with spiral baffling	>10,000	$0.027 (N_{Re})^{0.8} (N_{Pr})^{0.33} (\mu_b/\mu_w)^{0.14} (1 + 3.5D_c/D_e)$	This jacket is considered a special case of a helical coil if certain factors are incorporated into equations for calculating outside-film coefficients. In the equations at left and below, the equivalent heat transfer diameter $D_e$ , for a rectangular cross-section is equal to four times the width of the annular space, $w$ and $D_c$ is the mean or centerline diameter of the coil helix. Velocities are calculated from the actual cross-section of the flow area, $pw$ , where $p$ is the pitch of the spiral baffle, and from the effective mass flowrate, $W'$ , through the passage. The leakage around spiral baffles is considerable, amounting to 35–50% of the total mass flowrate. The effective mass flowrate is about 60% of the total mass flowrate to the jacket: $W' = 0.6 W$ . The $N_{Nu}$ for this equation should be expressed in terms of $D_e(N_{Nu} = h_j D_e/k)$ as should the Reynolds number ( $N_{Re} = D_e v \rho/\mu$ ), $k$ being thermal conductivity, $v$ being velocity, and $\rho$ being density.

**Table-B2**  
(continued)

Jacket type	Reynolds number ( $N_{Re}$ )	Nusselt number ( $N_{Nu}$ )	Remarks
Annular jacket with spiral baffling	$210 < N_{Re} < 10,000$		Use the above equations depending on the value of $N_{Re}$ .
Half-pipe coil jacket	Laminar flow	$18.6(N_{Re})^{0.33} (N_{Pr})^{0.33} (D_c/L)^{0.33} (\mu_b/\mu_w)^{0.14}$	When pipe coils are made with a semicircular cross-section, $D_e = \pi d_{ci}/2$ , where $d_{ci}$ is the inner diameter of the pipe, in feet. For calculating the velocity, the cross-sectional flow area equals $\pi d_{ci}^2/8$ . When pipe coils are made with a 120° central angle, $D_e = 0.0708 d_{ci}$ and the cross-sectional area equals $0.154(d_{ci})^2$ .
Half-pipe coil jacket	Turbulent flow	$0.027(N_{Re})^{0.2} (N_{Pr})^{0.33} (\mu_b/\mu_w)^{0.14} \times (1 + 3.5D_c/D_e)$	$D_c$ is the mean diameter of the coil.
Half-pipe coil jacket	Transition flow		Use the above equations depending of the value of $N_{Re}$ .
Dimple jacket	Laminar flow	$1.86(N_{Re})^{0.33} (N_{Pr})^{0.33} (D_c/L)^{0.33} (\mu_b/\mu_w)^{0.14}$	The equivalent diameter $D_e$ , in a dimpled jacket equals 0.66 in. the cross-sectional flow area equals 1.98 in. <sup>2</sup> per foot of vessel circumference.

Annular jacket with spiral baffling	<2,100	$1.86 (N_{Re})^{0.33} (N_{Pr})^{0.33} (D_e/L)^{0.33} (\mu_b/\mu_w)^{0.14}$	Same as the above. L is length of coil or jacket passage, ft
Annular jacket with spiral baffling	$2,100 < N_{Re} < 10,000$		Use the above equations depending on the value of $N_{Re}$
Annular jacket, no baffles	Laminar flow	$1.02 (N_{Re})^{0.45} (N_{Pr})^{0.33} (\mu_b/\mu_w)^{0.14} (D_e/L)^{0.4} \times (D_{jo}/D_{ji})^{0.8} (N_{Gr})^{0.05}$	$D_{ji}$ and $D_{jo}$ are the inside and outside diameters of the jacket respectively. For this equation, $D_e = D_{jo} - D_{ji}$ . The Grashof number $N_{Gr} = D_e^3 \rho g \beta \Delta t_G / \mu^2$ where $D_e$ is equivalent diameter, g is acceleration due to gravity, $\beta$ is coefficient of volumetric expansion, $\mu$ is viscosity, $\rho$ is density, and $\Delta t_G$ is the difference between the temperature at the wall and that in the bulk fluid. $N_{Gr}$ must be calculated from fluid properties at the bulk temperature.
Annular jacket with spiral baffling	<2,100	$1.86 (N_{Re})^{0.33} (N_{Pr})^{0.33} (D_e/L)^{0.33} (\mu_b/\mu_w)^{0.14}$	The Nusselt and Reynolds numbers must be calculated with $D_e$ as the diameter term.
Annular jacket, no baffles	Turbulent	$0.027 (N_{Re})^{0.8} (N_{Pr})^{0.33} (\mu_b/\mu_w)^{0.14} \times (1 + 3.5 D_e/D_c)$	For the equivalent heat transfer diameter for turbulent flow, use $D_e = [(D_{jo})^2 - (D_{ji})^2]/D_{ji}$ , where $D_{ji}$ and $D_{jo}$ are the inside and outside diameters of the jacket respectively. The cross-sectional flow area, $A_x = \pi[(D_{jo})^2 - (D_{ji})^2]/4$
Dimple jacket	Turbulent flow	$0.27 (N_{Re})^{0.8} (N_{Pr})^{0.33} (\mu_b/\mu_w)^{0.14}$	The coefficients are not very accurate due to turbulence created by the dimples in the flow steam.
Dimple jacket	Transition flow		Determine $N_{Nu}$ from the above equations depending on the value of $N_{Re}$ .

The dimensionless parameters:

$$\text{Reynolds number, } N_{Re} = \frac{\rho V D}{\mu} = \frac{\rho N D_A^2}{\mu}$$

where  $\rho$  = density  
 $V$  = velocity  
 $D$  = diameter  
 $D_A$  = impeller diameter  
 $N$  = rotational speed of the agitator  
 $\mu$  = viscosity

$$\text{Prandtl number, } N_{Pr} = \frac{C_p \mu}{k}$$

where  $C_p$  = specific heat  
 $\mu$  = viscosity  
 $k$  = thermal conductivity

$$\text{Nusselt number, } N_{Nu} = \frac{hD}{k}$$

where  $h$  = heat transfer coefficient  
 $D$  = diameter  
 $k$  = thermal conductivity

$$\text{Viscosity number, } \mu_b/\mu_w$$

where  $\mu_b$  = viscosity at the bulk fluid temperature  
 $\mu_w$  = viscosity at the wall surface temperature  
 $(\mu_b/\mu_w)^{0.14} \cong 1.0$  for water

$$\text{Grashof number, } N_{Gr} = \frac{D_e^3 \rho^2 g \beta \Delta t_G}{\mu^2}$$

where  $D_e$  = equivalent diameter  
 $\rho$  = density  
 $g$  = acceleration due to gravity  
 $\beta$  = coefficient of volumetric expansion  
 $\Delta t_G$  = difference between the temperature at the wall and that in the bulk fluid

## Appendix C-Thermo physical properties of matter

**Table C1-Thermo physical properties of selected metallic solids**

Composition	Melting Point (K)	Properties at 300 K				Properties at Various Temperatures (K)														
		$\rho$ (kg/m <sup>3</sup> )	$c_p$ (J/kg · K)	$k$ (W/m · K)	$\alpha \cdot 10^6$ (m <sup>2</sup> /s)	$k$ (W/m · K)/ $c_p$ (J/kg · K)														
						100	200	400	600	800	1000	1200	1500	2000	2500					
Gold	1336	19300	129	317	127	327	323	311	298	284	270	255								
Iridium	2720	22500	130	147	50.3	172	153	144	138	132	126	120	111							
Iron						90	122	133	138	144	153	161	172							
Pure	1810	7870	447	80.2	23.1	134	94.0	69.5	54.7	43.3	32.8	28.3	32.1							
Armco (99.75% pure)		7870	447	72.7	20.7	216	384	490	574	680	975	609	654							
Carbon steels																				
Plain carbon (Mn ≤ 1%, Si ≤ 0.1%)		7854	434	60.5	17.7			56.7	48.0	39.2	30.0									
AISI 1010		7832	434	63.9	18.8			487	559	685	1169									
Carbon-silicon (Mn ≤ 1%, 0.1% < Si ≤ 0.6%)		7817	446	51.9	14.9			58.7	48.8	39.2	31.3									
Carbon-manganese-silicon (1% < Mn ≤ 1.65%, 0.1% < Si ≤ 0.6%)		8131	434	41.0	11.6			487	559	685	1168									
Chromium (low) steels																				
½Cr-½Mo-Si (0.18% C, 0.65% Cr, 0.23% Mo, 0.6% Si)		7822	444	37.7	10.9			49.8	44.0	37.4	29.3									
1 Cr-½Mo (0.16% C, 1% Cr, 0.54% Mo, 0.39% Si)		7858	442	42.3	12.2			501	582	699	971									
1 Cr-V (0.2% C, 1.02% Cr, 0.15% V)		7836	443	48.9	14.1			42.2	39.7	35.0	27.6									
								487	559	685	1090									
								38.2	36.7	33.3	26.9									
								492	575	688	969									
								42.0	39.1	34.5	27.4									
								492	575	688	969									
								46.8	42.1	36.3	28.2									
								492	575	688	969									



**Table C2-thermo physical properties of gases at atmospheric pressure**

$T$ (K)	$\rho$ (kg/m <sup>3</sup> )	$c_p$ (kJ/kg · K)	$\mu \cdot 10^7$ (N · s/m <sup>2</sup> )	$\nu \cdot 10^6$ (m <sup>2</sup> /s)	$k \cdot 10^3$ (W/m · K)	$\alpha \cdot 10^6$ (m <sup>2</sup> /s)	$Pr$
<b>Oxygen (O<sub>2</sub>) (continued)</b>							
350	1.100	0.929	233.5	21.23	29.6	29.0	0.733
400	0.9620	0.942	258.2	26.84	33.0	36.4	0.737
450	0.8554	0.956	281.4	32.90	36.3	44.4	0.741
500	0.7698	0.972	303.3	39.40	41.2	55.1	0.716
550	0.6998	0.988	324.0	46.30	44.1	63.8	0.726
600	0.6414	1.003	343.7	53.59	47.3	73.5	0.729
700	0.5498	1.031	380.8	69.26	52.8	93.1	0.744
800	0.4810	1.054	415.2	86.32	58.9	116	0.743
900	0.4275	1.074	447.2	104.6	64.9	141	0.740
1000	0.3848	1.090	477.0	124.0	71.0	169	0.733
1100	0.3498	1.103	505.5	144.5	75.8	196	0.736
1200	0.3206	1.115	532.5	166.1	81.9	229	0.725
1300	0.2960	1.125	588.4	188.6	87.1	262	0.721
<b>Water Vapor (Steam)</b>							
380	0.5863	2.060	127.1	21.68	24.6	20.4	1.06
400	0.5542	2.014	134.4	24.25	26.1	23.4	1.04
450	0.4902	1.980	152.5	31.11	29.9	30.8	1.01
500	0.4405	1.985	170.4	38.68	33.9	38.8	0.998
550	0.4005	1.997	188.4	47.04	37.9	47.4	0.993
600	0.3652	2.026	206.7	56.60	42.2	57.0	0.993
650	0.3380	2.056	224.7	66.48	46.4	66.8	0.996
700	0.3140	2.085	242.6	77.26	50.5	77.1	1.00
750	0.2931	2.119	260.4	88.84	54.9	88.4	1.00
800	0.2739	2.152	278.6	101.7	59.2	100	1.01
850	0.2579	2.186	296.9	115.1	63.7	113	1.02

**TABLE C-3** Thermophysical Properties of Saturated Fluids

<i>Saturated Liquids</i>								
$T$ (K)	$\rho$ (kg/m <sup>3</sup> )	$c_p$ (kJ/kg · K)	$\mu \cdot 10^2$ (N · s/m <sup>2</sup> )	$\nu \cdot 10^6$ (m <sup>2</sup> /s)	$k \cdot 10^3$ (W/m · K)	$\alpha \cdot 10^7$ (m <sup>2</sup> /s)	$Pr$	$\beta \cdot 10^3$ (K <sup>-1</sup> )
<b>Engine Oil (Unused)</b>								
273	899.1	1.796	385	4280	147	0.910	47,000	0.70
280	895.3	1.827	217	2430	144	0.880	27,500	0.70
290	890.0	1.868	99.9	1120	145	0.872	12,900	0.70
300	884.1	1.909	48.6	550	145	0.859	6400	0.70
310	877.9	1.951	25.3	288	145	0.847	3400	0.70
320	871.8	1.993	14.1	161	143	0.823	1965	0.70
330	865.8	2.035	8.36	96.6	141	0.800	1205	0.70
340	859.9	2.076	5.31	61.7	139	0.779	793	0.70
350	853.9	2.118	3.56	41.7	138	0.763	546	0.70
360	847.8	2.161	2.52	29.7	138	0.753	395	0.70
370	841.8	2.206	1.86	22.0	137	0.738	300	0.70
380	836.0	2.250	1.41	16.9	136	0.723	233	0.70
390	830.6	2.294	1.10	13.3	135	0.709	187	0.70
400	825.1	2.337	0.874	10.6	134	0.695	152	0.70
410	818.9	2.381	0.698	8.52	133	0.682	125	0.70
420	812.1	2.427	0.564	6.94	133	0.675	103	0.70
430	806.5	2.471	0.470	5.83	132	0.662	88	0.70
<b>Ethylene Glycol [C<sub>2</sub>H<sub>4</sub>(OH)<sub>2</sub>]</b>								
273	1130.8	2.294	6.51	57.6	242	0.933	617	0.65
280	1125.8	2.323	4.20	37.3	244	0.933	400	0.65
290	1118.8	2.368	2.47	22.1	248	0.936	236	0.65
300	1114.4	2.415	1.57	14.1	252	0.939	151	0.65
310	1103.7	2.460	1.07	9.65	255	0.939	103	0.65
320	1096.2	2.505	0.757	6.91	258	0.940	73.5	0.65
330	1089.5	2.549	0.561	5.15	260	0.936	55.0	0.65
340	1083.8	2.592	0.431	3.98	261	0.929	42.8	0.65
350	1079.0	2.637	0.342	3.17	261	0.917	34.6	0.65
360	1074.0	2.682	0.278	2.59	261	0.906	28.6	0.65
370	1066.7	2.728	0.228	2.14	262	0.900	23.7	0.65
373	1058.5	2.742	0.215	2.03	263	0.906	22.4	0.65
<b>Glycerin [C<sub>3</sub>H<sub>8</sub>(OH)<sub>3</sub>]</b>								
273	1276.0	2.261	1060	8310	282	0.977	85,000	0.47
280	1271.9	2.298	534	4200	284	0.972	43,200	0.47
290	1265.8	2.367	185	1460	286	0.955	15,300	0.48
300	1259.9	2.427	79.9	634	286	0.935	6780	0.48
310	1253.9	2.490	35.2	281	286	0.916	3060	0.49
320	1247.2	2.564	21.0	168	287	0.897	1870	0.50

**TABLE C.3** *Continued*

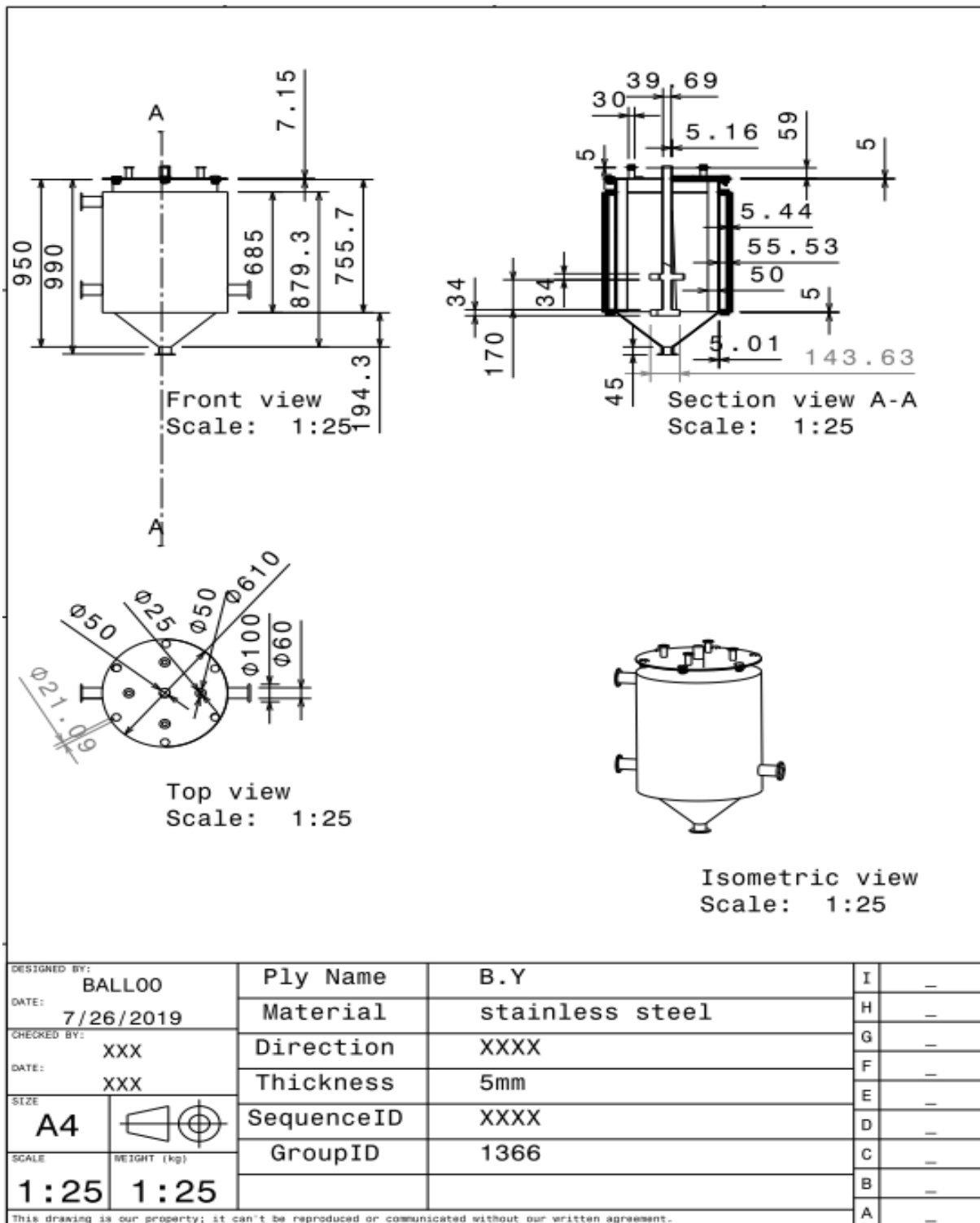
<i>Saturated Liquid-Vapor, 1 atm<sup>b</sup></i>					
Fluid	$T_{sat}$ (K)	$h_{fg}$ (kJ/kg)	$\rho_f$ (kg/m <sup>3</sup> )	$\rho_g$ (kg/m <sup>3</sup> )	$\sigma \cdot 10^3$ (N/m)
Ethanol	351	846	757	1.44	17.7
Ethylene glycol	470	812	1111 <sup>c</sup>	—	32.7
Glycerin	563	974	1260 <sup>c</sup>	—	63.0 <sup>c</sup>
Mercury	630	301	12,740	3.90	417
Refrigerant R-134a	247	217	1377	5.26	15.4
Refrigerant R-22	232	234	1409	4.70	18.1

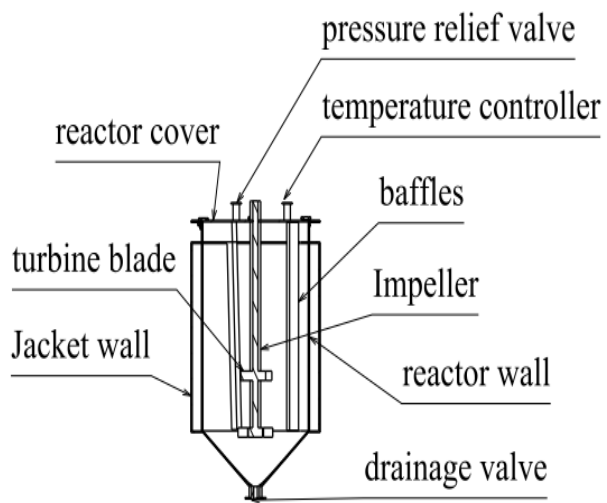
TABLE C.4 Thermophysical Properties of Saturated Water<sup>a</sup>

Temperature, <i>T</i> (K)	Pressure, <i>p</i> (bars) <sup>b</sup>	Specific Volume (m <sup>3</sup> /kg)		Heat of Vaporization, <i>h<sub>fg</sub></i> (kJ/kg)	Specific Heat (kJ/kg·K)		Viscosity (N·s/m <sup>2</sup> )		Thermal Conductivity (W/m·K)		Prandtl Number		Surface Tension, <i>σ<sub>l</sub></i> ·10 <sup>3</sup> (N/m)	Expansion Coefficient, <i>β<sub>l</sub></i> ·10 <sup>6</sup> (K <sup>-1</sup> )	Temperature, <i>T</i> (K)
		<i>v<sub>f</sub></i> ·10 <sup>3</sup>	<i>v<sub>g</sub></i>		<i>c<sub>p,f</sub></i>	<i>c<sub>p,g</sub></i>	<i>μ<sub>f</sub></i> ·10 <sup>6</sup>	<i>μ<sub>g</sub></i> ·10 <sup>6</sup>	<i>k<sub>f</sub></i> ·10 <sup>3</sup>	<i>k<sub>g</sub></i> ·10 <sup>3</sup>	<i>Pr<sub>f</sub></i>	<i>Pr<sub>g</sub></i>			
273.15	0.00611	1.000	206.3	2502	4.217	1.854	1750	8.02	569	18.2	12.99	0.815	75.5	-68.05	273.15
275	0.00697	1.000	181.7	2497	4.211	1.855	1652	8.09	574	18.3	12.22	0.817	75.3	-32.74	275
280	0.00990	1.000	130.4	2485	4.198	1.858	1422	8.29	582	18.6	10.26	0.825	74.8	46.04	280
285	0.01387	1.000	99.4	2473	4.189	1.861	1225	8.49	590	18.9	8.81	0.833	74.3	114.1	285
290	0.01917	1.001	69.7	2461	4.184	1.864	1080	8.69	598	19.3	7.56	0.841	73.7	174.0	290
295	0.02617	1.002	51.94	2449	4.181	1.868	959	8.89	606	19.5	6.62	0.849	72.7	227.5	295
300	0.03531	1.003	39.13	2438	4.179	1.872	855	9.09	613	19.6	5.83	0.857	71.7	276.1	300
305	0.04712	1.005	29.74	2426	4.178	1.877	769	9.29	620	20.1	5.20	0.865	70.9	320.6	305
310	0.06221	1.007	22.93	2414	4.178	1.882	695	9.49	628	20.4	4.62	0.873	70.0	361.9	310
315	0.08132	1.009	17.82	2402	4.179	1.888	631	9.69	634	20.7	4.16	0.883	69.2	400.4	315
320	0.1053	1.011	13.98	2390	4.180	1.895	577	9.89	640	21.0	3.77	0.894	68.3	436.7	320
325	0.1351	1.013	11.06	2378	4.182	1.903	528	10.09	645	21.3	3.42	0.901	67.5	471.2	325
330	0.1719	1.016	8.82	2366	4.184	1.911	489	10.29	650	21.7	3.15	0.908	66.6	504.0	330
335	0.2167	1.018	7.09	2354	4.186	1.920	453	10.49	656	22.0	2.88	0.916	65.8	535.5	335
340	0.2713	1.021	5.74	2342	4.188	1.930	420	10.69	660	22.3	2.66	0.925	64.9	566.0	340
345	0.3372	1.024	4.683	2329	4.191	1.941	389	10.89	668	22.6	2.45	0.933	64.1	595.4	345
350	0.4163	1.027	3.846	2317	4.195	1.954	365	11.09	668	23.0	2.29	0.942	63.2	624.2	350
355	0.5100	1.030	3.180	2304	4.199	1.968	343	11.29	671	23.3	2.14	0.951	62.3	652.3	355
360	0.6209	1.034	2.645	2291	4.203	1.983	324	11.49	674	23.7	2.02	0.960	61.4	679.9	360
365	0.7514	1.038	2.212	2278	4.209	1.999	306	11.69	677	24.1	1.91	0.969	60.5	707.1	365
370	0.9040	1.041	1.861	2265	4.214	2.017	289	11.89	679	24.5	1.80	0.978	59.5	728.7	370
373.15	1.0133	1.044	1.679	2257	4.217	2.029	279	12.02	680	24.8	1.76	0.984	58.9	750.1	373.15
375	1.0815	1.045	1.574	2252	4.220	2.036	274	12.09	681	24.9	1.70	0.987	58.6	761	375
380	1.2869	1.049	1.337	2239	4.226	2.057	260	12.29	683	25.4	1.61	0.999	57.6	788	380
385	1.5233	1.053	1.142	2225	4.232	2.080	248	12.49	685	25.8	1.53	1.004	56.6	814	385
390	1.794	1.058	0.980	2212	4.239	2.104	237	12.69	686	26.3	1.47	1.013	55.6	841	390
400	2.455	1.067	0.731	2183	4.256	2.158	217	13.05	688	27.2	1.34	1.033	53.6	896	400
410	3.302	1.077	0.553	2153	4.278	2.221	200	13.42	688	28.2	1.24	1.054	51.5	952	410
420	4.370	1.088	0.425	2123	4.302	2.291	185	13.79	688	29.8	1.16	1.075	49.4	1010	420
430	5.699	1.099	0.331	2091	4.331	2.369	173	14.14	685	30.4	1.09	1.10	47.2		430

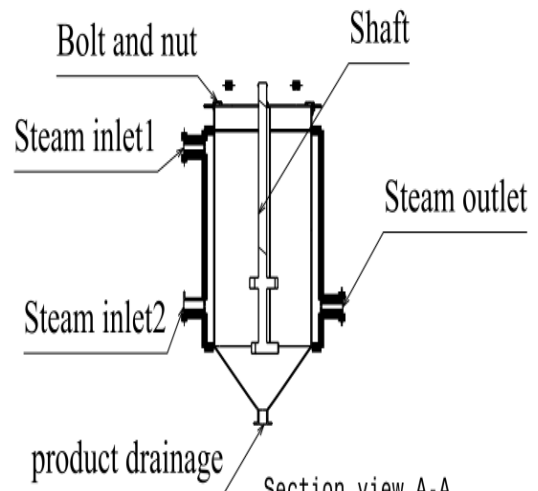
## Appendix D: Design specification of reactor

Table D-Detail drawing of jacketed reactor with agitator





Section view A-A  
 Scale: 1:20



Section view A-A  
 Scale: 1:20