CHAPTER 1

INTRODUCTION

Thermochemical conversion of biomass to gaseous and fuels is an attractive alternative route to meet energy demands on a sustainable basis. The goal of gasification is to break down the biomass polymers to gases, which are called syngas composed of CO, CO_2, H_2 and CH_4. Biomass mainly consists of three types of carbohydrate polymers which are lignin, cellulose and hemicellulose. Inconsistency in structure and composition of biomass polymers, and their unknown reaction pathways during the thermal degradation process, lead to complexities in predicting the composition and flowrates of the final product gas from gasification (McKendry, 2002). Factors influencing gasification process can be divided into two categories that are characteristics of biomass, design of the gasification system and operating conditions of the gasification system. Biomass characteristics include proximate analysis, ultimate analysis, energy content and particle size distribution. While the operating conditions of the gasification system include biomass flowrate, steam to biomass ratio, air fuel ratio, temperatures of air and steam of the gasifier. In this paper, operating conditions of the gasification are taken into account while developing a model to predict composition and properties of the product gases and determine the optimum operating parameters. Since ASPEN Plus contains a large property database for conventional compounds and convergence algorithms for solving minimization problems, it can be used to develop a gasification model.

1.1 Background of Study

Biomass fuel derived from organic matter on a renewable basis is among the largest sources of energy in the world, third only to coal and oil (Bapat, 1997). Biomass adsorbs CO_2 from the atmosphere during photosynthesis, and the CO_2 is then returned to the environment through combustion. Because of this cycle, biomass is CO_2 neutral, making it an advantageous fuel source and a dominant choice for replacement of fossil fuels as the concern of global warming increases. For gasification of fossil fuels emissions can

be drastically reduced when compared to traditional power plants. This is due to increased efficiency and because the fuel input has been converted to gaseous form, making it possible to remove the contaminants that cause the emissions prior to combustion. Energy security is of utmost importance and is vital for any country's continued economic growth. According to a recent study, oil and gas prices are set to double by 2050 (Rezaiyan, 2005). Global energy demand is also set to more than double by the middle of the century. Biomass gasification coupled with other renewable energy options would cut dependency on fossil fuels and would help to ensure energy security.

1.2 Problem Statement

A limited supply of fossil fuels and an ever growing demand for energy sources have intensified the search for alternative renewable energy sources. Energy from biomass has the potential to meet the energy demands of the world given its abundant availability on a sustainable basis (Demirbas, 2001). Design parameters and operating conditions of the gasifier highly influence the resulting syngas composition and its calorific value. It is difficult to manually determine the optimum values of the parameters and operating conditions that result in higher performance and safe operation of the unit. There is also lack of time to do experiment many times with different value of variable in order to determine which parameter at what value will give the optimum result. Thus, there is a need to predict the output of the gasification system by means of ASPEN Plus Simulation Software, which can give the optimum result of syngas composition. The feedstock to be used in this simulation is Oil Palm Fronds (OPF). Development of process using ASPEN Plus is easier, save time, less expensive, customizable, self-documenting and can handle complex processes.

1.3 Objective

The goals of this project were to model the gasification process in a downdraft gasifier using OPF as a feedstock for the optimum operating conditions that would result in the best composition of syngas by means of ASPEN Plus software. Overall, the specific objectives of this project were to:

1. Develop an ASPEN Plus-based gasification model to predict the product composition for a given biomass characteristics.
2. Determine the best operating conditions that would result in the best composition of syngas.

1.4 Scope of Study

This project involved computer simulation by ASPEN Plus Simulator Software. A model of gasification process in downdraft gasifier for OPF is developed to determine the optimum operating conditions that would result in the best composition of the syngas. Data from past experiments or simulation is used to calibrate this model. Based on these simulations, the parameters of the gasification of OPF are characterized.

The energy crisis spectrum which was a constant of the last decades, urged the need to develop tools appropriate for the design or retrofit of complex industrial processes. This project gives benefit to researchers in biomass field by lowering the cost of doing experiment because ASPEN Plus is widely used throughout the work and experimental work is carried out only to verify the simulation if needed. In addition, gasification operators achieve the best gasification performance by knowing the optimum operating condition that would result in the best composition of syngas.

CHAPTER 2
LITERATURE REVIEW AND THEORY

OPF is one of the most abundant agricultural byproduct in Malaysia with an estimated availability of 36 million tones annually. OPF is obtained during replanting as well as during harvesting and pruning. On average, there are 24 fronds per palm tree. The weight of OPF varies from 15 kg to 20 kg depending on age of the palm tree. Most of the OPFs are left to rod on the ground between the oil palm trees with the purpose of soil conservation, erosion control and ultimately for long term benefit of nutrient recycling.

2.1 Biomass's development

In Malaysia, there is a rapid increase in energy demand as the nation is to become a fully developed country by 2020. Besides that, the country has very limited energy reserves which can only last for 30-40 year whereby it will become net oil importer by 2040 (Zahari, 2004). By venturing into possibility of developing biomass into alternative energy, there are some advantages and disadvantages. Among the advantages are biomass is a renewable energy, while it is sustainable and environmentally friendly. Besides that, there is abundant supply and it is an untapped energy. But due to lack of relevant technology and uneconomical factor, biomass industry faces a great hindrance to progress in this country.

2.2 Gasification of Carbonaceous Materials

Gasification is a process that converts carbonaceous materials, such as coal, petroleum, or biomass, into carbon monoxide, hydrogen and carbon dioxide. The resulting gas mixture is called synthesis gas or known as syngas. Syngas consists primarily of H_2, CO, CO_2 and CH_4. Syngas is combustible and often used as a fuel source or as an intermediate for the production of other chemicals. Gasification is a very efficient method for extracting energy from many different types of organic materials and also has applications as a clean waste disposal technique (Rajvanshi, 1986). The gasification process involves 4 main reactions which are drying, pyrolysis, combustion/oxidation and

reduction. The first process is drying, in which the material at the upper side of the gasifier will be heated up by the heat from the hearth zone. This process will eliminate the moisture content of the feed up to 160°C. Pyrolysis occurs at the bottom of drying zone where volatile gases are released from the dry biomass. These gases are non-condensable vapors (e.g. methane, carbon-monoxide) and condensable vapors (various tar compounds) and the residuum from this process will be mainly activated.

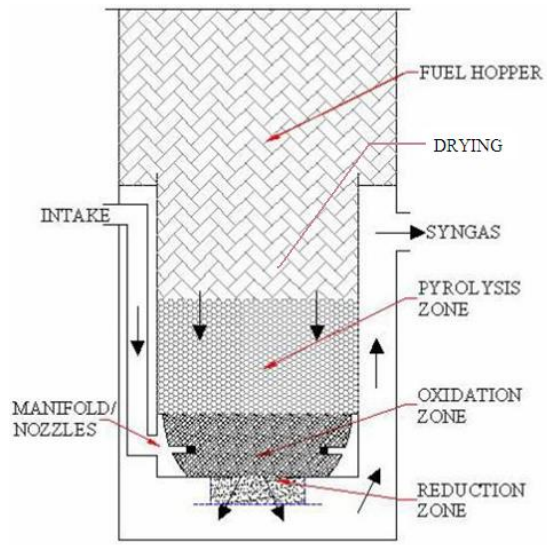


Figure 2.1: Typical process in a downdraft gasifier (Forestry Department, 1986)

The combustion or oxidation process occur where the remaining char is combusted (reaction with oxygen) to provide heat, carbon dioxide, carbon monoxide and water vapor. The general reaction of the process is described as (Reed, 2005):

$$C + O_2 \Leftrightarrow CO_2 \quad (2.1)$$

$$H_2 + 1/2O_2 \Leftrightarrow H_2O \quad (2.2)$$

The heat produced from the combustion process will be transported by convection and radiation to heat up the feed at the upper side. After combustion, reduction process is carried out. The chemical process is described as (Reed, 2005):

$$C + CO_2 \Leftrightarrow 2CO \quad (2.3)$$

$$C + H_2O \Leftrightarrow CO + H_2 \quad (2.4)$$

$$CO + H_2 \Leftrightarrow CO + H_2O \quad (2.5)$$

$$C + 2H_2 \Leftrightarrow CH_4 \quad (2.6)$$

$$CO + 3H_2 \Leftrightarrow CH_4 + H_2O \quad (2.7)$$

The process of reduction is the simultaneous reaction of char, carbon dioxide and water vapor from the combustion process to produce producer gas that mainly composed of carbon monoxide and hydrogen. Equations (2.3) and (2.4), which are the main reactions of reduction, show that reduction requires heat. Therefore the gas temperature will decrease during reduction.

2.3 Composition of Synthesis gas

Syngas (from Synthesis gas) is the name given to a gas mixture that contains varying amounts of carbon monoxide and hydrogen generated by the gasification of a carbon containing fuel to a gaseous product with a heating value (Mckendry, 2001).

The factors that affect the syngas composition include temperature distribution in fuel bed, average gas residence time, air velocity and residence time distribution. These factors are dependent on the geometry and the gasifier design. Besides all those geometrical and design factors, the syngas composition also depends on physical properties of the biomass, in this case the OPF itself. Researches and simulation will be conducted in order to find the relationship between the OPF physical properties and the gasifier optimum operating conditions.

2.4 Types of Gasifier

A gasifier is equipment to converts solid fuel into the producer gas through a thermo-chemical process. The gas produced mainly used for heat or power generation applications. The overall thermal efficiency of this process is more than 75% and the producer gas normally contains CO, H_2, N_2, CO_2 and CH_4 (Ghandour, 2005). There are four main types of gasifier available for commercial uses which are the updraft, downdraft, cross draft and fluidized bed gasifier.

2.4.1 Updraft Gasifier

Updraft gasifier is the simplest gasifier among the other types of gasifier. The material will be feed at the top of the gasifier and will moves down due to gasification and ash removal process. The air will be supplied from the bottom and the gas will leaves at the top and that is the reason why it is called updraft gasifier. The zones inside the gasifier from the top to bottom are the drying zone, pyrolysis zone, reduction zone and the combustion zone, placed at the bottom part of the reactor (Reed, 2005).

Major advantages of updraft gasifier are its simplicity, high char burn, high efficiencies and low gas exit temperature. The variation of fuel also can be tolerated and small size particle can be used. The major drawback is that the amount of tar and pyrolysis product is high since the gas is not combusted. This has been major concern to environmental issue as the tar content can bring effects on environment and good purification system is required to overcome the problem.

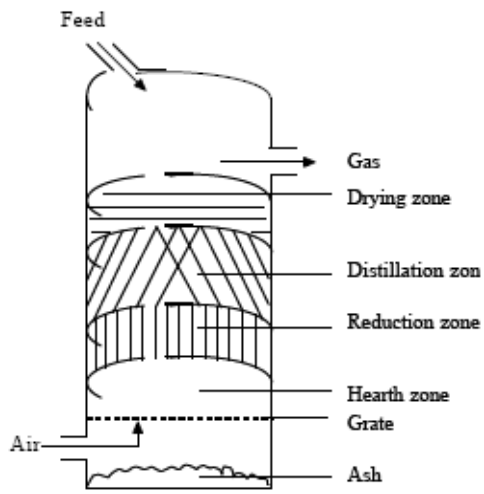


Figure 2.2: Sketch of Typical Updraft Gasifier (Ghandour, 2005).

2.4.2 Crossdraft gasifier

The gasification process in crossdraft gasifier results in very high temperature which is nearly 1500°C and even higher in the hearth zone which can lead to material problems. Advantages of the system lie in the very small scale at which it can be operated due to

very high gas cleaning train. A drawback is the minimal tar-converting capability, resulting in the need for high charcoal. (Reed, 2005)

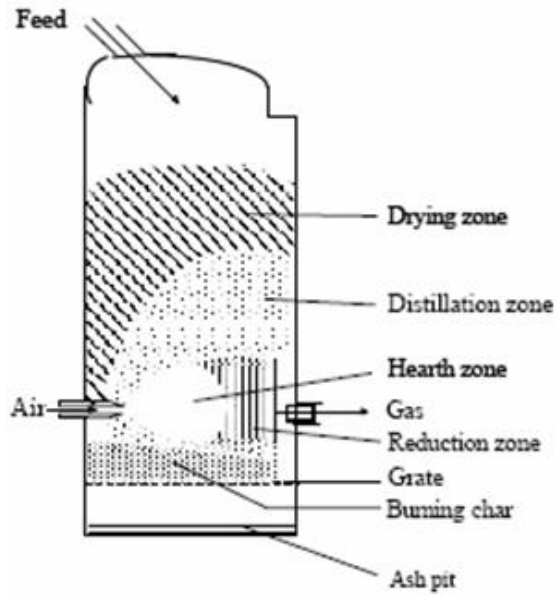


Figure 2.3: Sketch of Typical Cross draft Gasifier (Ghandour, 2005).

2.4.3 Fluidized bed gasifier

This gasifier is is suitable for larger capacity and designed to overcome the operational problem of high ash content. The gasification temperature is lower compared to fixed bed gasifier around 750 to 900°C (Reed, 2005). The fuel is fed into hot sand which is instate of suspension or circulating. The bed behaves more or less like a fluid and it is characterized by high turbulence. Fuel particles mix quickly with the bed material creates fast pyrolysis and large amount of pyrolysis gas.

The advantages of the gasifier are the ability to changes in fuel characteristic and deal with fine grained material with high as content or low bulk density. Relatively low ash melting pointes are allowed due to the low reaction temperature.

The disadvantages are formation of high content of tar and dust in producer gas and incomplete carbon burn out. The high producer gas temperature containing alkali metal in the vapor state and there is complex gasifier operation because of the need to control

the supply of both air supply and solid fuel. Power consumption is needed for the compression of the gas stream (Reed, 2005).

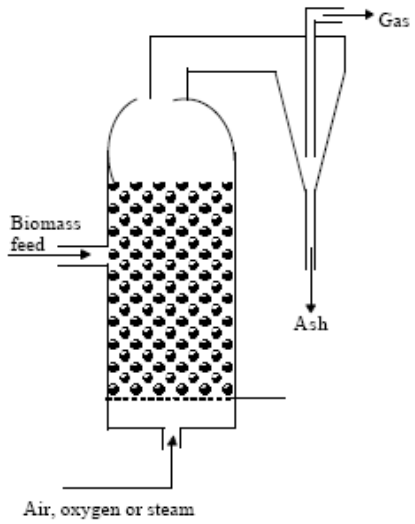


Figure 2.4: Sketch of Typical Fluidized bed Gasifier (Ghandour, 2005).

2.4.4 Downdraft Gasifier

This gasifier is applicable for medium and large scale of power generation ranging from 80 kW up to 500 kW or more. Some lab scale gasifiers are available in 5 kW (Reed, 2005). The feedstock is fed at the top and the air for the combustion is fed either from the top or side. The gas leaves at the bottom with same direction as material movement that is the reason why it is called downdraft gasifier. The zones are slightly different from the up draft type as the reduction zone is occur at the bottom of the gasifier.

The main advantage of down draft is the producer gas will content low amount of tar as the gas will flow through combustion and reduction zone prior exit at the outlet. However, the residence time is the important factor to consider ensuring the tar is combusted through the hottest zone. In each particular design, other features are includes to realize a high conversion rate of the pyrolysis gas (Reed, 2005).

2.5 Modelling with ASPEN Plus software.

Perfect contact between gas and solid, along with a high degree of turbulence, improves heat and mass transfer characteristics, and enhances the ability to control temperature, and increases heat storage and volumetric capacity (Strehler, 2009). The ASPEN PLUS process simulator has been used by different investigators to simulate coal conversion. For examples include integrated coal gasification combined cycle (IGCC) power plants (Philip, 1986), atmospheric fluidized bed combustor processes (Douglas, 1990) and coal gasification simulation (Lee, 1992).

However, the work that has been done on biomass gasification is limited. Mansaray in 2000 used ASPEN PLUS to simulate rice husk gasification based on material balance, energy balance, and chemical equilibrium relations. Because of the high amount of volatile material in biomass and the complexity of biomass reaction rate kinetics in fluidized beds, they ignored the char gasification and simulated the gasification process by the assumption that biomass gasification follows Gibbs equilibrium. In a typical atmospheric fluidized bed gasifier, feed, together with bed material, are fluidized by the gasifying agents, such as air and/or steam, entering at the bottom of the bed. The product gas resulting from the gasification process is fed to a gas–solid separator (i.e., cyclone) to separate solid particles carried by exhaust gas.

2.5.1 Types of Reactor block use in ASPEN Plus

There are two types of block that is usually used in modelling simulation using ASPEN Plus that are Yield Reactor, RYIELD and Gibbs Reactor, R-GIBBS. RYIELD models a reactor by specifying reaction yields of each component. This model is useful when reaction stoichiometry and kinetics are unknown and yield distribution data or correlations are available. While R-GIBBS models a single-phase chemical equilibrium, or simultaneous phase and chemical equilibrium by minimizing Gibbs free energy, subject to atom balance constraints. This model is useful when temperature and pressure are known and reaction stoichiometry is unknown.

2.5.2 Type of run using in ASPEN Plus for Modelling

There are three types of run used in modelling simulation diagram using ASPEN Plus software that are Data Regression, Property Analysis and Property Estimation. The description of the types of run is shown in the table below.

Table 2.1: Run types that are used to run ASPEN Plus software Simulation (ASPEN Plus user guide, 2003)

Run Type	Description
Data Regression	A standalone data regression runs. Can contain property constant estimation and property analysis calculation
Property Analysis	A standalone property analysis run. Can contain property constant estimation and assay data analysis calculations.
Property Estimation	A standalone property constant estimation run.

The function of Data Regression is to fit physical property model parameters required by ASPEN Plus to measured pure component and other mixture data. ASPEN Plus cannot perform data regression in a flowsheet run. Property Analysis function to perform property analysis by generating tables of physical property values when do not want to perform a flowsheet simulation in the same run. The function of roperty Estimation is to estimate property parameters when a flowsheet simulation in the same run is not required.

2.5.3 Experiment Data Adapt form Past Work Paper

Below are the Ultimate Analysis and Proximate Analysis of Oil Palm Fronds adapted from Balamohan in 2007. These data is used as the input to run the simulation in this project.

Table 2.2: Experimental Result for Ultimate Analysis (Balamohan, 2007).

	Carbon	**Hydrogen**	**Nitrogen**	**Sulphur**
Ultimate Analysis	42.55%	5.48%	2.18%	0.11%

Table 2.3: Experimental Result for Proximate Analysis (Balamohan, 2007).

	Moisture	**Volatile Matter**	**Fixed Carbon**	**Ash**
Proximate Analysis	4.0%	51.3%	39.7%	6.3%

CHAPTER 3

METHODOLOGY AND PROJECT WORK

3.1 Methodology flow Chart

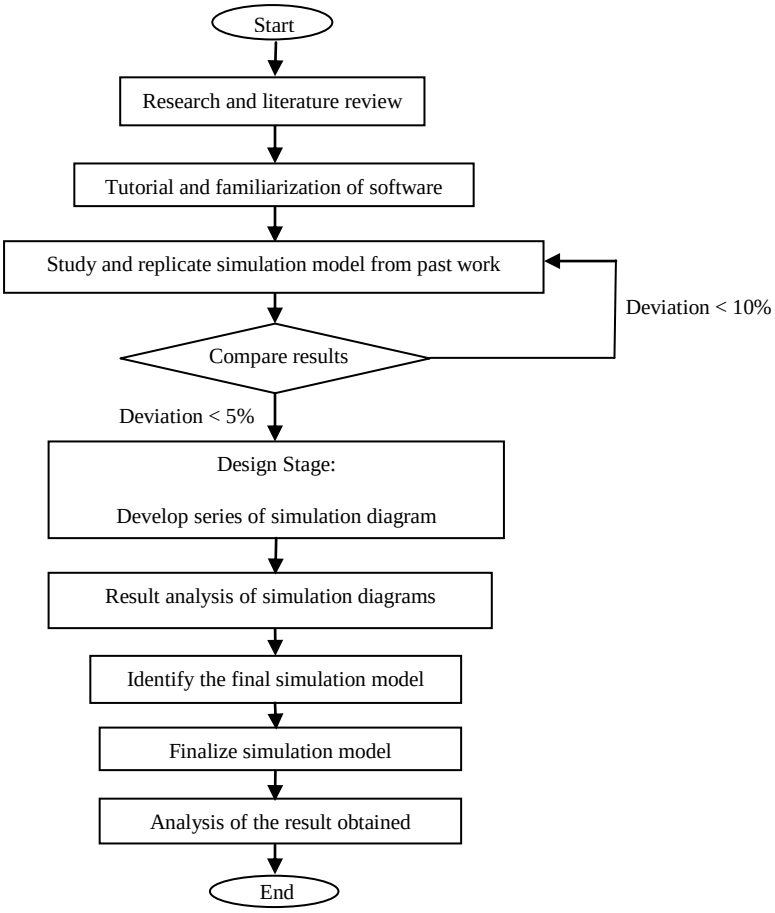


Figure 3.1: Project Methodology Flow chart.

A further research through available resources such as internet, journals, previous related FYP dissertation and discussion with fellow students and supervisor was conducted to have a clearer view of the topic. As this project required coordination with postgraduate student, there are a lot of discussions held from time to time. Since this software required lot of practice to get familiar and better understanding, many tutorials was done. All the results were compared with those shown in the tutorial manual. After that, a model form past work adapted from literature was replicated. The result was compared and analyzed.

3.2 Key milestone and Gantt Chart

The key milestone in this project is reached when optimum operating conditions in the best composition of the syngas has been determined. The Gantt Charts for the project are shown in Figure 3.2 and Figure 3.3. These Gantt Chart shows the work planned and summarized the elements of project for 2 semester.

No.	Activities/Week	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	Selection of project topic														
2	Data gathering and research on topic														
3	Literature review on research project topic														
4	Submission of preliminary report				21st Aug 09										
5	Do tutorials and get familiar with ASPEN Plus Software														
6	Research on OPF relation with gasification optimum conditions.														
7	Submission of progress report 1 and Seminar								11th Sept 09						
8	Research on optimum composition of Syngas														
9	Replication of past work from literature														
10	Submission of interim report													26th Oct 09	
11	Oral presentation														9th Nov 09

Figure 3.2: Gantt Chart for Semester I

No.	Activities/Week	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	Literature review on research project topic														
2	Design Stage: Develop a series of simulation diagram														
3	Analysis of all the result obtained														
4	Submission of progress report 1				10th Feb 10										
5	Compare the result of the simulation diagrams														
6	Finalize the selected simulation model														
7	Submission of progress report 2								15th Mac 10						
8	Seminar								25th Mac 10						
9	Further analysis of final simulation model														
10	Poster Exhibition & Dissertation											1st Apr 10			
11	Preparation for oral presentation														
12	Hardbound dissertation														

Figure 3.3: Gantt Chart for Semester II

3.3 ASPEN Plus software Tools

The main tool required to implement this project is ASPEN Plus Simulator Software. ASPEN Plus allows a user to build a process model and then simulate the model without tedious calculations. It can be used to model many processes involving solids. Some of the solids processing applications that can be modeled by the software include:

- Bayer process
- Coal gasification
- Hazardous waste incineration
- Iron ore reduction
- Zinc smelting/roasting

ASPEN Plus was selected for modelling the gasifier. It is a steady state chemical process simulator, which was developed to evaluate synthetic fuel technologies.

3.3.1 Reasons to Use ASPEN Plus simulation software.

The introduction of solids to a chemical process can affect the process in many ways. In all cases, the heat and mass balances of the process are changed, even if the solid essentially passes through the process as an inert component. Simulation of the heat and mass balances of a solids process requires physical property models suitable for solid components. The physical property models used to characterize a liquid may not be relevant for solids.

In addition to specialized physical property models for solid components, accurate representation of the solids particle size distribution is required for some processes. For example, the separation efficiency of a cyclone is highly dependent on the size of the particles entrained in the feed gas.

ASPEN Plus has thermodynamic models, and rigorous unit operation models built-in. The simulator can easily handle complex processes with solids. Even with all of the built-in capabilities, ASPEN Plus is customizable when necessary. Very importantly, ASPEN Plus is a simulator that is self-documenting and easy to understood by anyone knowledgeable in the software. Finally, it is commercially supported and widely accepted by the process industries.

3.3.2 ASPEN Plus Modelling Approach

General Assumption in the ASPEN Plus Model

The following are general assumptions that were considered in modelling the biomass gasification process (Xiong, 2004):

- Biomass devolatilization takes place instantaneously and volatile products mainly consist of CO, CO_2, H_2 and CH_4 and H_2O.
- All the gases are uniformly distributed within the emulsion phase.
- Particles are spherical and of uniform size and the average diameter remain constant during the gasification, based on the shrinking core model.

3.3.3 Equivalent Ratio, ER

Equivalence ratio is defined as follow:

$$\mathrm{ER} = \frac{\text{Weight oxygen (air)/weight dry biomass}}{\text{Stoichiometric oxygen (air)/biomass ratio}} \tag{3.1}$$

3.3.4 General Step to work on ASPEN Plus

ASPEN Plus uses unit operation blocks, which are models of specific process operations. These blocks are placed on a flow sheet, specifying material and energy streams. An extensive built in physical properties database is used for the simulation

calculations. ASPEN Plus has the capability to incorporate FORTRAN code, an imperative computer programming language into the model. This feature is utilized for the definition of non-conventional fuels, for example biomass, specific coals and for ensuring the system operates within user defined limits and constraints. The development of a model in ASPEN Plus involves the following steps:

1. Stream class specification and property method selection.
2. System component specification from databank.
3. Defining the process flow sheet (unit operation blocks, connecting material and energy streams).
4. Specifying feed streams (flow rate, composition, and thermodynamic condition).
5. Specifying unit operation blocks (thermodynamic condition and chemical reactions)

3.3.5 Modelling Project Simulation Diagram using ASPEN Plus

Modelling of the project simulation diagram using ASPEN Plus has been started and now about 60 percent completed. In carrying out the modelling, some hypotheses is made. The following hypotheses were considered to draw the model:

1. The process is in steady state.
2. Char only contains carbon and ash
3. This process was supposed to occur instantaneously at equilibrium with volatile products mainly made of CO, CO_2, H_2 and CH_4 and H_2O.
4. Tars are assumed to be negligible in the syngas.

3.3.6 Reactor Specification and Characteristic

<u>Equilibrium Reactor, R-Equilb</u>

R-Equilb models reactors when some or all reactions reach equilibrium. R-Equilb can calculate single phase chemical equilibrium, or simultaneous phase and chemical

equilibria. R-Equilb calculates equilibrium by solving stoichiometric chemical and phase equilibrium equations. R-Equilb is used to model a reactor when reaction stoichiometry is known and some or all reactions reach chemical equilibrium. R-Equilb allows restricted chemical equilibrium specifications for reactions that do not reach equilibrium. R-Equilb can model one- and two-phase reactors.

Flowsheet Connectivity for R-Equilb

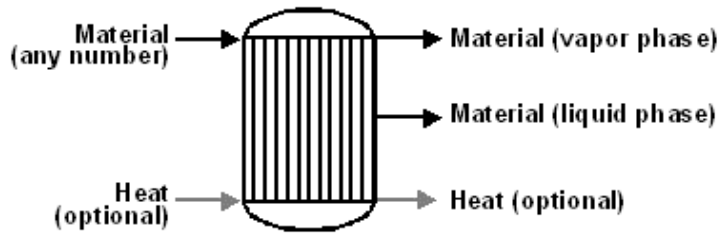


Figure 3.4: Schematic diagram of equilibrium reactor

Material Streams Description :

Inlet is equal to material stream while outlet are one material stream for the vapor phase and one material stream for the liquid phase. The net heat duty is the sum of the inlet heat streams minus the actual (calculated) heat duty.

Gibbs Reactor, R-Gibbs

Calculation and mathematical formula involve in the R-GIBBS reactor

General chemical reaction for R-GIBBS reactor:

$$0 = \Sigma \nu_i A_i \tag{3.2}$$

where ν_i is the stoichiometric coefficient for component A_i, with $\nu_i > 0$ for products and $\nu_i > 0$ for reactants. Approximate interpretation of Gibbs free energy:

$$\Delta G^0 = \Delta H^0 - T\Delta S^0 \tag{3.3}$$

where ΔH^0 is the enthalpy of formation and ΔS^0 is the entropy of formation. While ΔH^0 and ΔS^0 are also temperature dependent, they are only slightly so. Taking natural logarithms get:

$$\ln K_p = -\frac{\Delta H^0}{RT} + \frac{\Delta S^0}{R} \tag{3.4}$$

Thus, the slope of a ln (K_p) versus 1/T plot is best interpreted as $-\Delta H^0/R$ and its intercept as $\Delta S^0/R$. concentration-based equilibrium constant K_C of an ideal-gas reaction (Wilcox, 2007):

$$\ln K_C = -\frac{\Delta H^0}{RT} + \frac{\Delta S^0}{R} - \sum \nu_i \ln(RT) \tag{3.5}$$

3.4 General Description of Project Work and Activities.

This project work consists of 2 parts as below:

PART 1 : Duplication of past work paper.

PART II : Modelling of simulation diagram for biomass gasification process.

This below section will discuss in detail about the respective part.

3.4.1 PART I : Duplication of Past Work paper

The simulation model form Mehrdokht et al in 2008 is replicated to verify that the work done and future work by the author in modelling processes using ASPEN Plus is reliable. The objective of that past work paper is to develop simulation capable of predicting the steady-state performance of an atmospheric fluidized bed gasifier. The products of homogeneous reactions are defined by Gibbs equilibrium, and reaction rate kinetics is used to determine the products of char gasification. 3 parameters are used to determine their effect to syngas composition. The parameters are:

1) Temperature.

2) Equivalent Ratio.
3) Biomass Particle Size.

The graph between the three parameters and component of syngas that are H_2, CO, CO_2 and CH_4 is plotted. Then, the result obtained is compared with the result form past work paper. Percentage of error between author's and past work is calculated. The results of the duplication are shown in Chapter 4.

3.4.2 PART II : Modelling of Biomass Gasification Process.

In designing the simulation diagram, there are many ways, choice and combination of element that can be done to achieve the objective of this project. Therefore, to develop this project, a series of simulation diagram had been constructed and further improved from time to time to obtained the most reliable simulation diagram. For the analysis of the result, sensitivity analysis is carried out. The operating parameters used are temperature, pressure and air fuel ratio and their effect on syngas composition are presented. The details of the three simulation diagrams are discussed as below.

3.4.2.1 General Information about Variation of Simulation Diagrams

First simulation diagram and second simulation diagram has the same block diagram used and flowsheet stream connection except that for second simulation diagram Gibbs Reactor is replace by Equilbrium Reactor to perform combustion and reduction process. The third simulation diagram have similar diagram with first simulation diagram with addition of Separator before the product is combusted and reduced. So, to make it clear, these three diagram is given more specific name as below:

First Simulation Diagram = R-Equilb Model
Second Simulation Diagram = R-Gibbs Model
Third Simulation Diagram = R-Gibbs Separator Model

This variation is done mostly to identify which component is suitable to be used for biomass gasification process that will produce the most accurate result. Since ASPEN Plus is not specifically design for biomass gasification process only, it is important to make sure that the only accurate component is used to simulate the gasification process. Later, the result obtained will be compared later with past work.

3.4.2.2 First Simulation Diagram (R-Equilb Model)

In the first simulation diagram, feed that is OPF will be supply to Yield Reactor, RYIELD. RYIELD is responsible for the process of drying the OPF and then follow by the process of pyrolisis. In this reactor, biomass is converted into its constituting components including carbon, hydrogen, oxygen, sulfur, nitrogen, and ash by specifying the yield distribution according to the biomass ultimate analysis.

Then the product from Yield Reactor that is symbolized by stream S1 will flow to the Equilibrium Reactor, R-EQUILB. In this reactor, all the chemical process occurs need to be specified, that is the chemical equation involved. So in R- EQUILB, combustion will takes place with the following equation:

$$C + O_2 \Leftrightarrow CO_2 \tag{3.6}$$

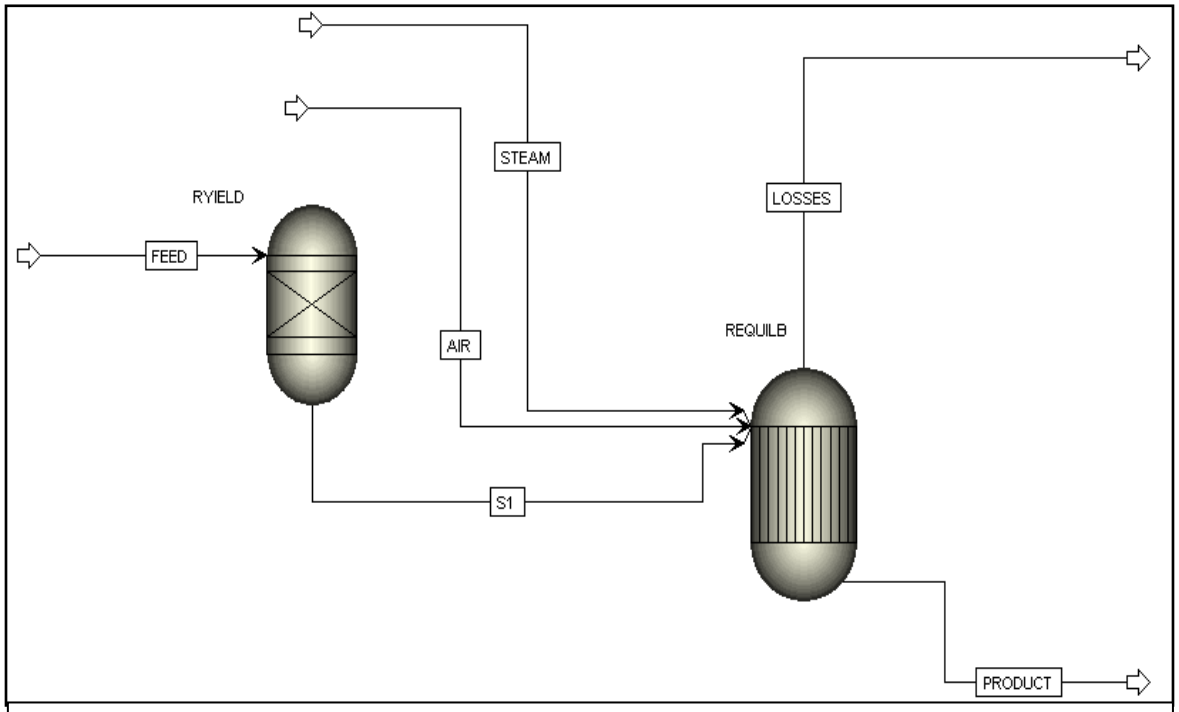
$$H_2 + 1/2O_2 \Leftrightarrow H_2O \tag{3.7}$$

After that, process of reduction will occur that follow the chemical equation as below:

$$C + CO_2 \Leftrightarrow 2CO \tag{3.8}$$

$$C + H_2O \Leftrightarrow CO + H_2 \tag{3.9}$$

Then, the final product is obtained and any losses such as heat and impurities will flow out through this reactor. The schematic of the first simulation is shown in Figure 3.5.



Legend:

- FEED : OPF feedstock
- RYEILD: Yield Reactor
- REQUILB: Equilibrium Reactor
- S1: Product after drying and pyrolisis
- AIR: Air supply
- STEAM: Steam supply
- LOSSES: Heat losses
- PRODUCT: Final product

Figure 3.5: Simulation diagram for R-Equilb Model.

3.4.2.3 Second Simulation Diagram (R-Gibbs Model)

The second simulation diagram is the improvement from the first simulation diagram. It has the similarities with the first simulation diagram except R-EQUILB is replace by Gibbs Reactor, R-GIBBS. R-EQUILB and R-GIBBS is falls under category of equilibrium reactor and have nearly the same function except for the operation process and input to be used. After the feedstock has undergone the process of drying and pyrolisis by RYIELD, the product is flow to R-GIBBS. R-GIBBS was used for volatile partial combustion, based on the assumption that volatile reactions follow the Gibbs equilibrium. Steam is also supplied to R- GIBBS for the process of reduction. Then final product is obtained from this reactor. The schematic of the second simulation is shown in Figure 3.6.

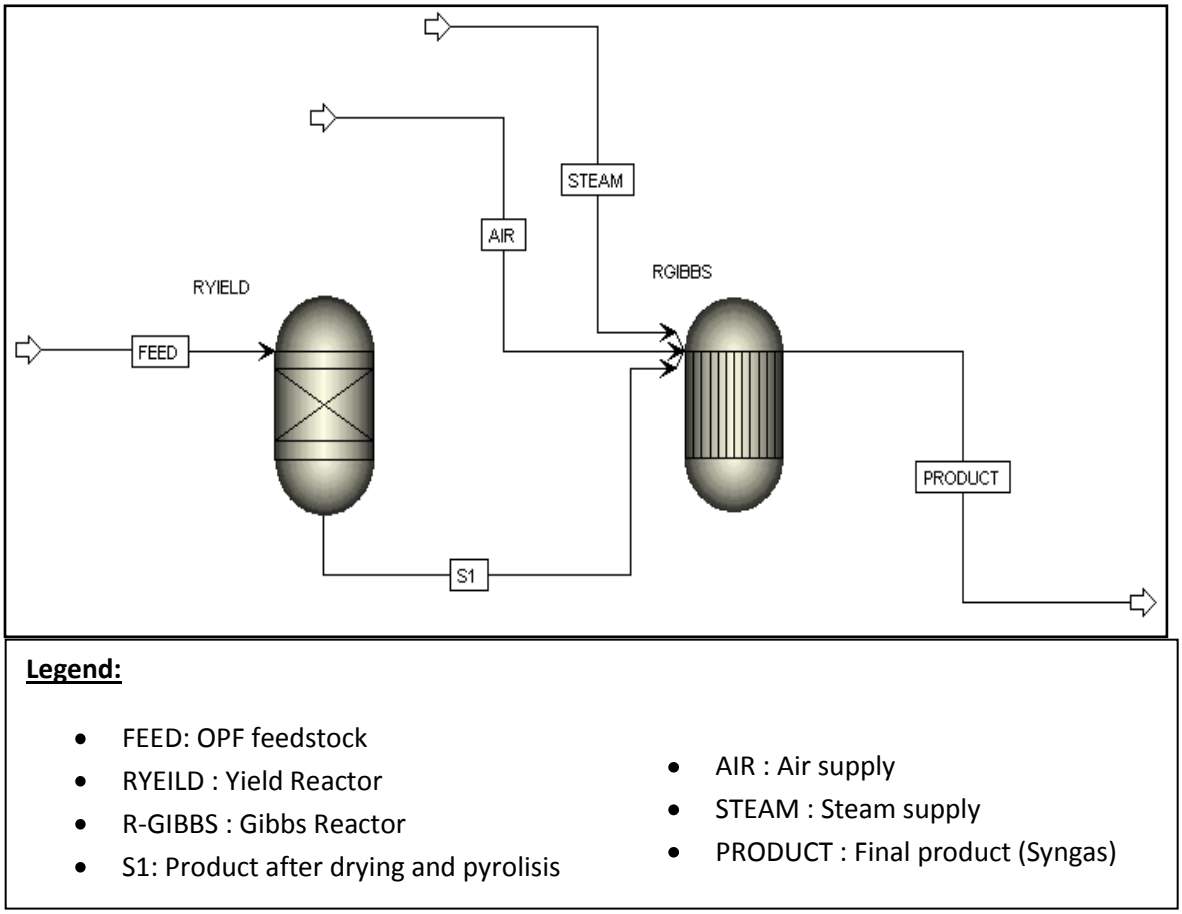
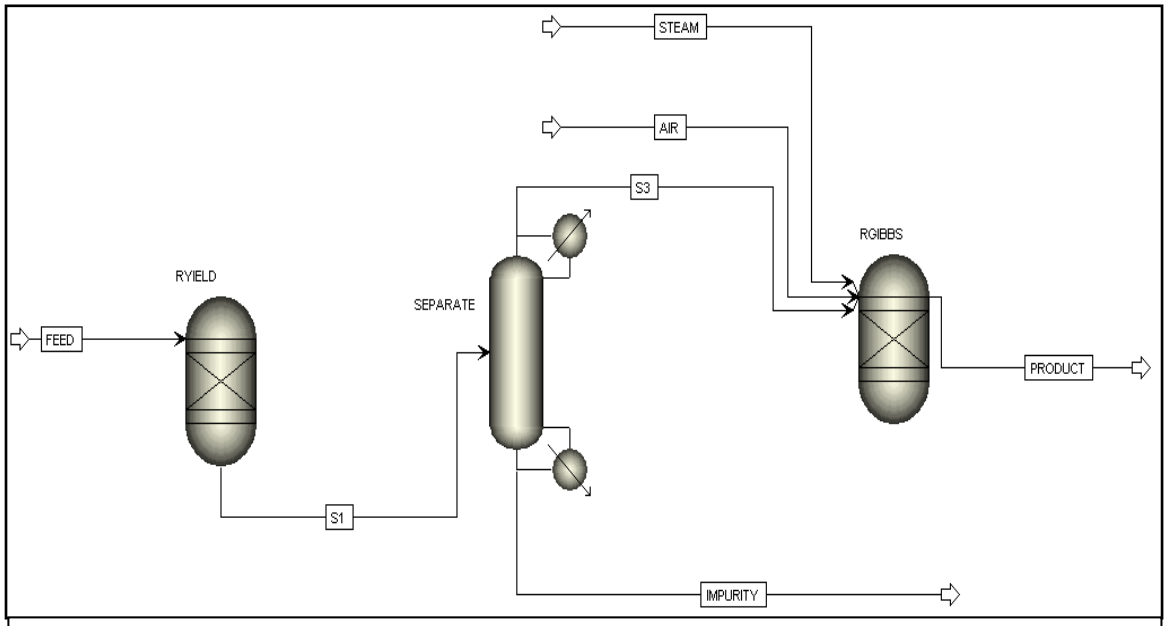


Figure 3.6: Simulation diagram for R-Gibbs Model.

3.4.2.4 Third Simulation Diagram (R-Gibbs Separator Model)

Third simulation diagram have nearly the same with the second simulation diagram except that the separation column or Separator is installed after the product have undergone drying and pyrolisis at RYIELD. The function of separator is to separate between carbon and other impurities like nitrogen sulfide, ash, nitrogen gas and sulphur. So only carbon will allow to flow to Gibbs Reactor for combustion and reduction process and the other component will allow flowing out to another stream. The results obtained tend to be more accurate. The schematic of the third simulation is shown in Figure 3.7.



Legend:

- FEED: Biomass feedstock (OPF)
- RYEILD: Yield Reactor
- R-GIBBS: Gibbs Reactor
- S1: Product after drying and pyrolisis
- S3 : Carbon stream
- IMPURITY : Ash, N_2, H_2S
- SEPARATE: Separator
- AIR: Air supply
- LOSSES: Heat losses
- PRODUCT: Final product (Syngas)

Figure 3.7: Simulation diagram for R-Gibbs Separator Model.

3.4.2.5 Detail Work Step in Modeling Biomass Gasification Process

1. The unit to be used is specified.

In this simulation, Metric Unit is used and below is the detail of the specification with respective unit:

Parameter	Unit
Volume-flow	cum/hr
Enthalpy-flow	gcal/hr

Pressure	bar
Temperature	^{o}C
Volume	cum
Head	meter
Mole-density	kmol/cum
Mass-density	kg/cum
Mole-enthalpy	kcal/mol
Mass-enthalpy	kcal/kg
Heat	gcal

2. The stream function is defined.

The global stream class is MIXCISLD (Mix Conventional Inert Solid). The CISOLID substream (Conventional Inert Solid) is used for homogeneous solids that have a defined molecular weight. The NC substream (Nonconventional) is used for heterogeneous solids that have no defined molecular weight. Both the CISOLID substream and the NC substream give the option of including a Particle Size Distribution (PSD) for the substream. The Solids application type default stream class, MIXCISLD, is insufficient for this simulation since NC substream will be used.

3. The flow basis and stream and report composition is set.

For this project Flow basis for input is Mole and Stream report composition is Mole flow.

4. The entire component involved in the simulation is listed.

The componenst for this simulation are H_2, O_2, CO, CO_2, H_2O, N_2, CH_4, S, C, biomass (oil palm fronds) and ash.

5. The connectivity on flowsheet is set.

Block R-Yield in = Feed. Block R-Yield out=S1

Block R-Gibbs in=S3. Block R-Gibbs out= Product

Block separator in=S1. Block separator out = S3 and Impurity.

6. The property of Air Stream is specified.

Parameter	**Value**
Temperature	65°C
Pressure	1.05 bar
Volume-flow	0.567 cum
Mole-fraction	O_2 0.21 / N_2 0.79

7. The property of Stream Feed (OPF) is specified.

Substream function is NCPSD (NonConventional Particle Size Distribution). Temperature is 25 ^{o}C and pressure is 1.05 bar. Component attribute proxanal for OPF is specified as below:

Moisture	Volatile Matter	Fixed Carbon	Ash
4%	51.3%	38%	6.3%

Component attribute ultanal for OPF is specified as below:

Carbon	Hydrogen	Nitrogen	Sulphur
42.55%	5.48%	2.18%	0.11%

8. The property of Steam Stream is specified.

Parameter	Value
Temperature	154°C
Pressure	1.05 bar
Mass-flow	0.8 cum
Mole-fraction of H_2O	1.0

9. The property of Block R-Yield is specified.

Parameter Temperature is 25 ^{o}C and pressure is 1.05 bar. Proxanal analysis for moisture is set to equal to zero. *DRY_REAC Setup Reactions* sheet is used to simulate drying process. This block models the drying of OPF. The following equation is the chemical reaction for drying:

$$CH_{1.54}O_{0.88} \text{ (wet OPF)} \rightarrow 0.81\ H_2O + C \tag{3.5}$$

The reaction indicates that 1 mole of OPF reacts to form 0.81 mole of water. The material balance equations for this process define relations between the following quantities:

- Water content of the feed OPF
- Fractional conversion of OPF to water
- Water content of the dried OPF

$$OPF\text{-}IN * \frac{H20-IN}{100} = OPF\text{-}OUT * \frac{H20-OUT}{100} + OPF\text{-}IN * CONV \tag{3.6}$$

$$OPF\text{-}IN = OPF\text{-}OUT + OPF\text{-}IN * CONV \tag{3.7}$$

Where: *OPF-IN* = Mass flow rate of OPF in stream WET-OPF

OPF-OUT = Mass flow rate of OPF in stream IN-DRIER

H2O-IN = Percent moisture in the OPF in stream WET-OPF

CONV = Fractional conversion of OPF to H2O in the block R-YIELD

Equation 3.6 is the material balance for water, and equation 3.7 is the overall material balance. These equations can be combined to yield equation 3:

$$\text{CONV} = \frac{\text{H20IN} - \text{H2OOUT}}{100 - \text{H20OUT}} \tag{3.8}$$

Next, the Calculator block specifies the moisture content of the dried OPF and calculates the corresponding conversion of OPF to water. For pyrolisis process, Proxanal analysis for volatile matter is set to equal to zero.

10. The property of Block R-Gibbs is specified

Parameter temperature equal to 660 ^{o}C, pressure equal to 1.05 bar and constant heat is supply for combustion process. Chemical equations involved for this reactor are as below:

For combustion :

$$C + O_2 \Leftrightarrow CO_2$$

$$H_2 + 1/2O_2 \Leftrightarrow H_2O$$

For Reduction :

$$C + CO_2 = 2CO$$

$$C + H_2O = CO + H_2$$

11. The results are analyzed using sensitivity analysis.

Sensitivity 1 = Temperature

Parameter	Value
Minimum temperature	350°C
Maximum temperature	1000°C
Increment	50°C
Output	Variation of mole composition of syngas

Sensitivity 2 = Pressure

Parameter	Value
Minimum pressure	0.0 bar
Maximum pressure	7.0 bar
Increment	0.5 bar
Output	Variation of mole composition of syngas

Sensitivity 3 = Air Fuel Ratio, AFR

Parameter	Value
Minimum AFR	0.00
Maximum AFR	0.70
Increment	0.05
Output	Variation of mole composition of syngas

Shown in Figure 3.8 and Figure 3.9 is the overview of the simulation diagram when fit in to the real downdraft gasifier.

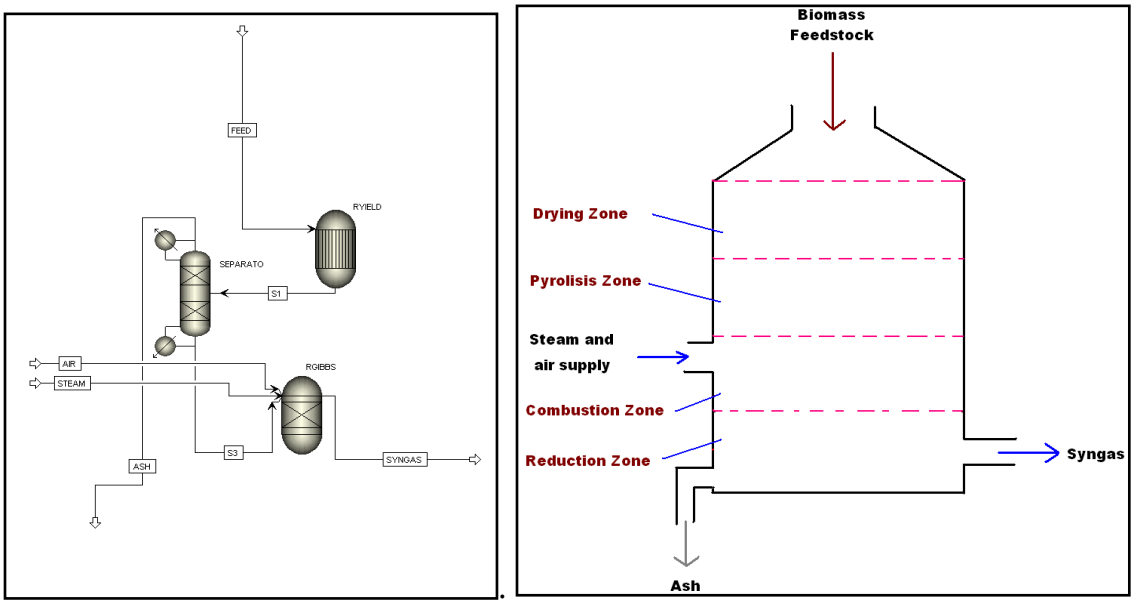


Figure 3.8 : Simulation Model of Gasification Process and respective gasifier diagram.

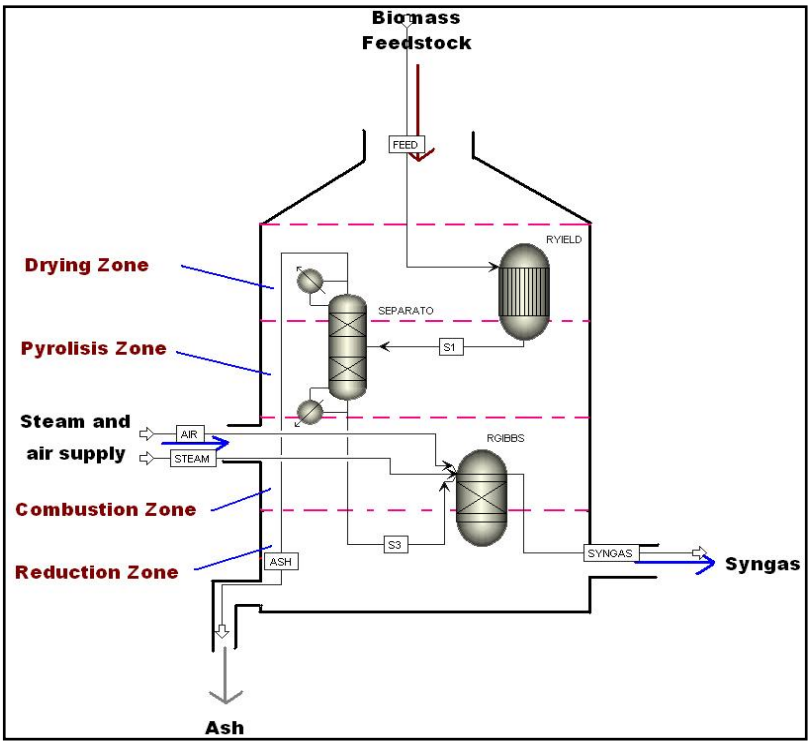


Figure 3.9: Simulation Model of Gasification Process when fit in gasifier.

CHAPTER 4

RESULT AND DISCUSSION

4.1 PART 1 : Result for Duplication of Past Work Paper.

The purpose of duplication of past work paper is to verify that the work done and future work by the author in modelling processes using ASPEN Plus is reliable. The objective of that past work paper is to develop simulation capable of predicting the steady-state performance of an atmospheric fluidized bed gasifier. The graph of temperature, equivalent ratio and biomass particle size versus and component of syngas are shown in Figure 4.1 until Figure 4.12.

4.1.1 Effect of Reactor Temperature on Composition of Syngas at biomass feed rate of 0.445kg/h, air flow rate of 0.5 m^3/h and steam flow rate of 1.2 kg/h.

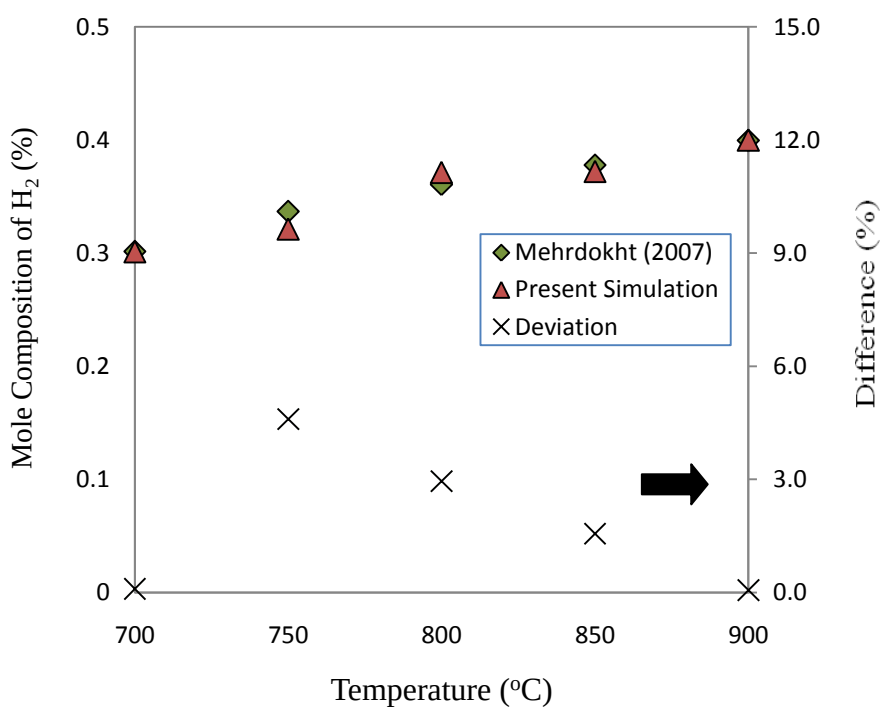


Figure 4.1: Variation of mole composition of H_2 with temperature and the difference.

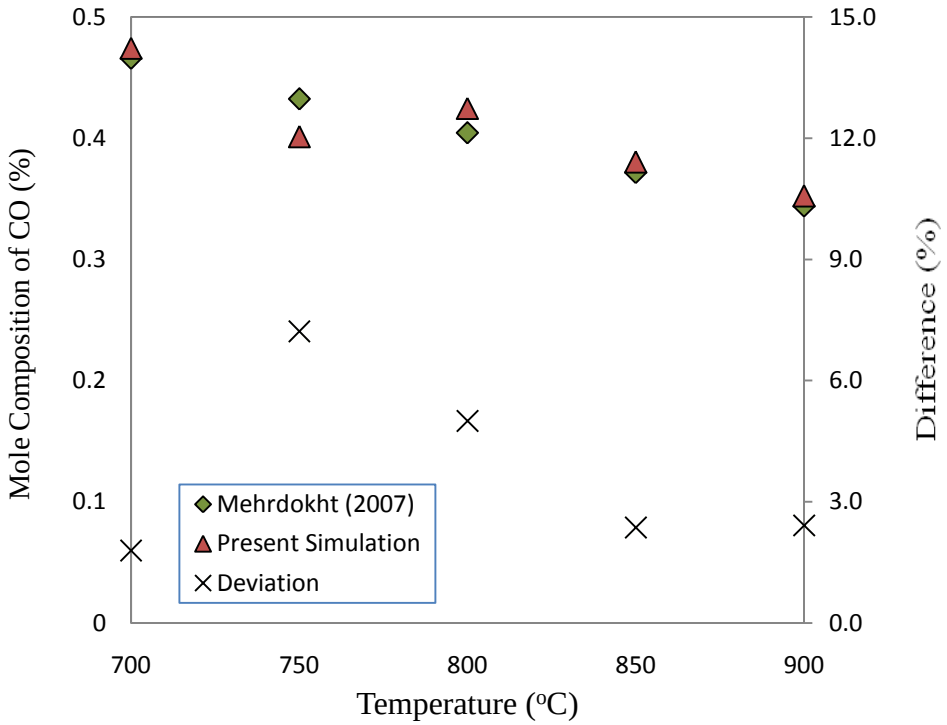


Figure 4.2: Variation of mole composition of CO with temperature and the difference.

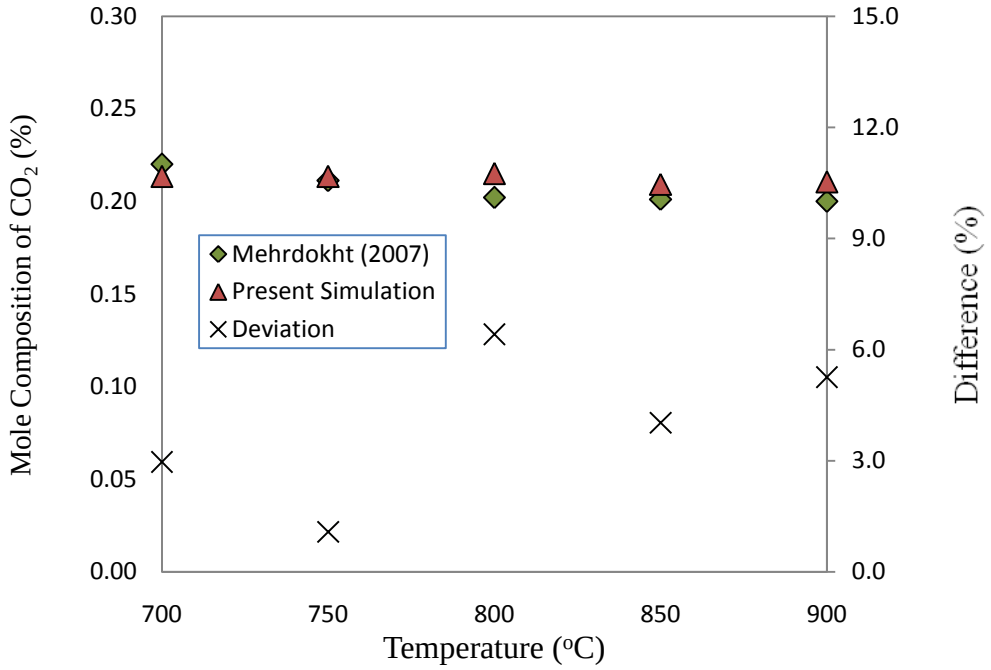


Figure 4.3: Variation of mole composition of CO_2 with temperature and the difference.

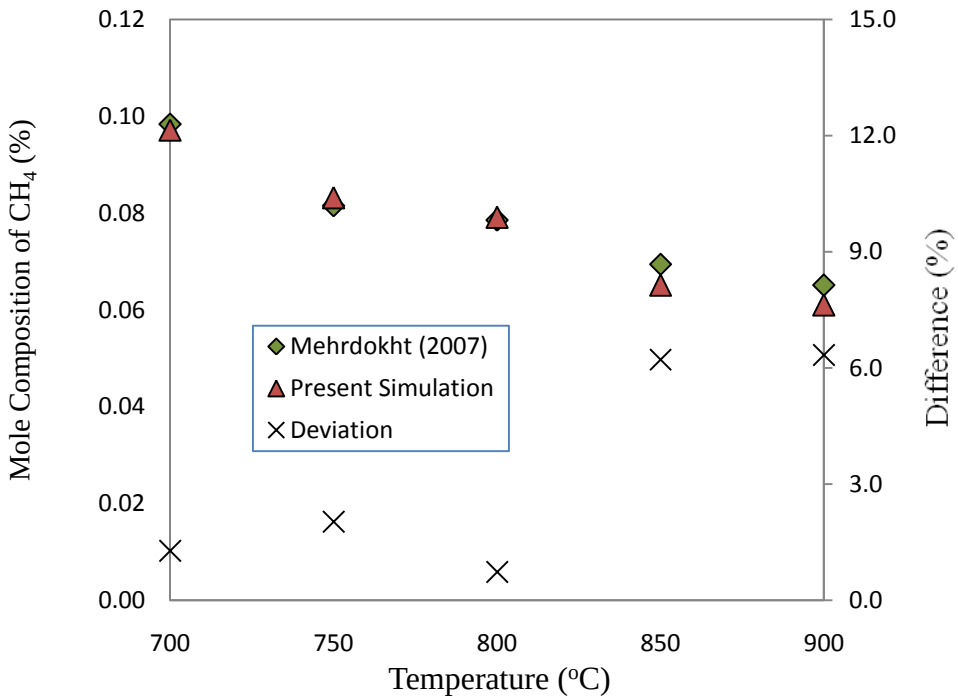


Figure 4.4: Variation of mole composition of CH_4 with temperature and the difference.

4.1.2 Effect of Equivalent Ratio on Composition of Syngas at biomass feed rate of 0.445kg/h, air flow rate of 0.5 m^3/h and steam flow rate of 1.2 kg/h.

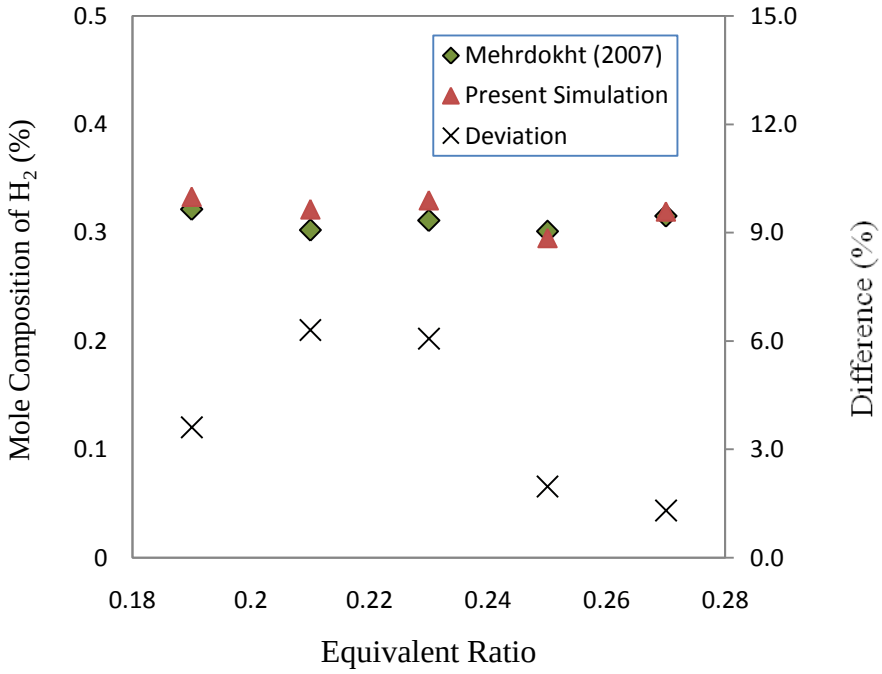


Figure 4.5: Variation of mole composition of H_2 with equivalent ratio and the difference.

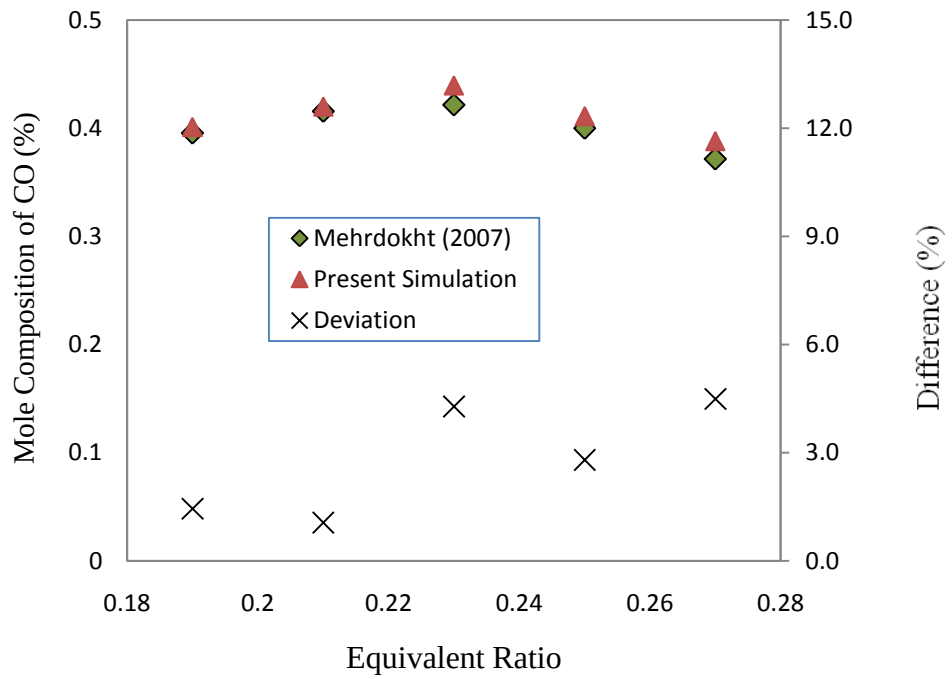


Figure 4.6: Variation of mole composition of CO with equivalent ratio and the difference.

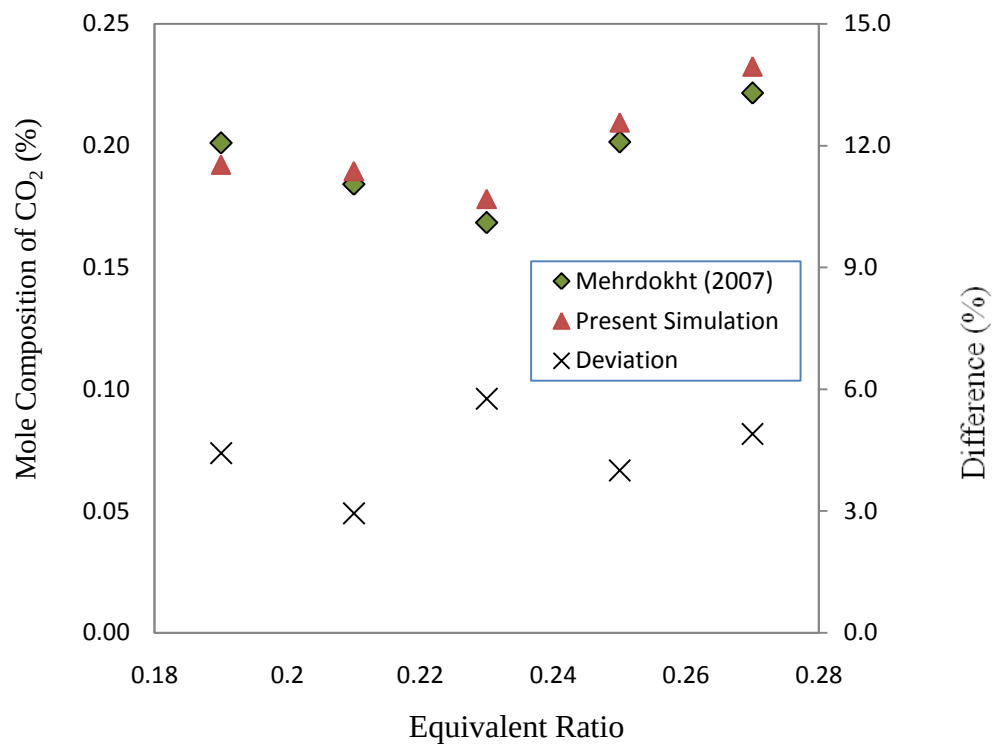


Figure 4.7: Variation of mole composition of CO_2 with equivalent ratio and the difference.

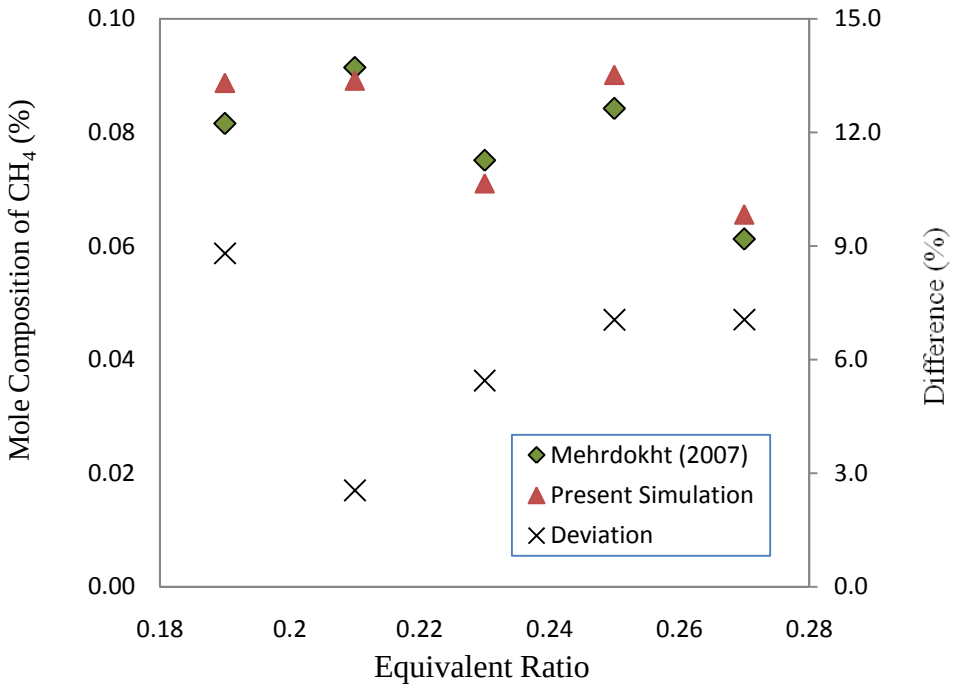


Figure 4.8: Variation of mole composition of CH_4 with equivalent ratio and the difference

4.1.3 Effect of Biomass Particle Size on Composition of Syngas at biomass feed rate of 0.445kg/h, air flow rate of 0.5 m^3/h and steam flow rate of 1.2 kg/h.

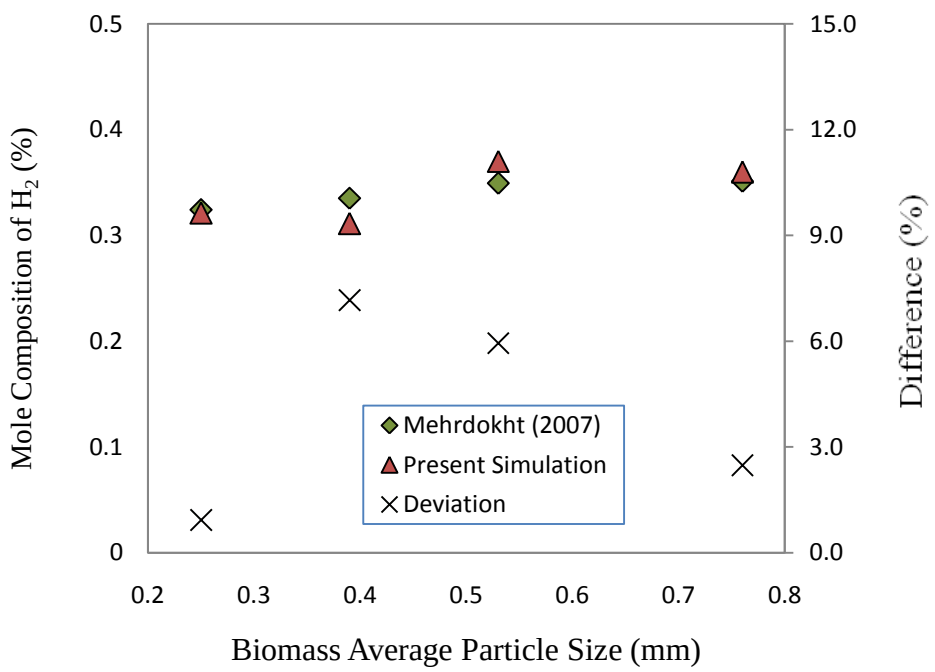


Figure 4.9: Variation of mole composition of H_2 with biomass particle size and the difference.

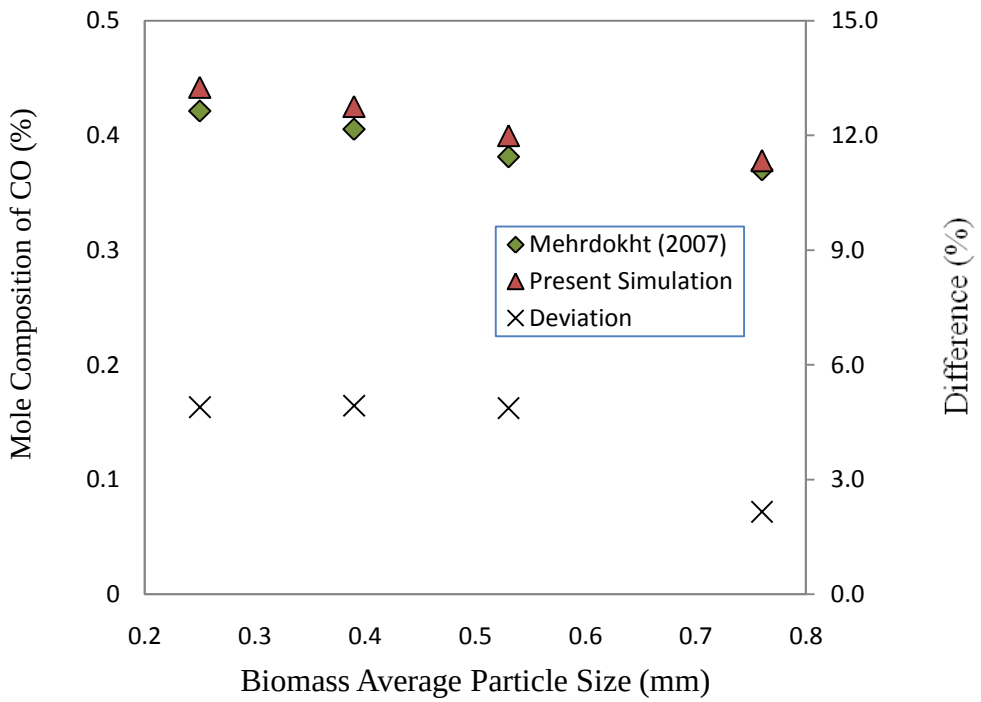


Figure 4.10: Variation of mole composition of CO with biomass particle size and the difference.

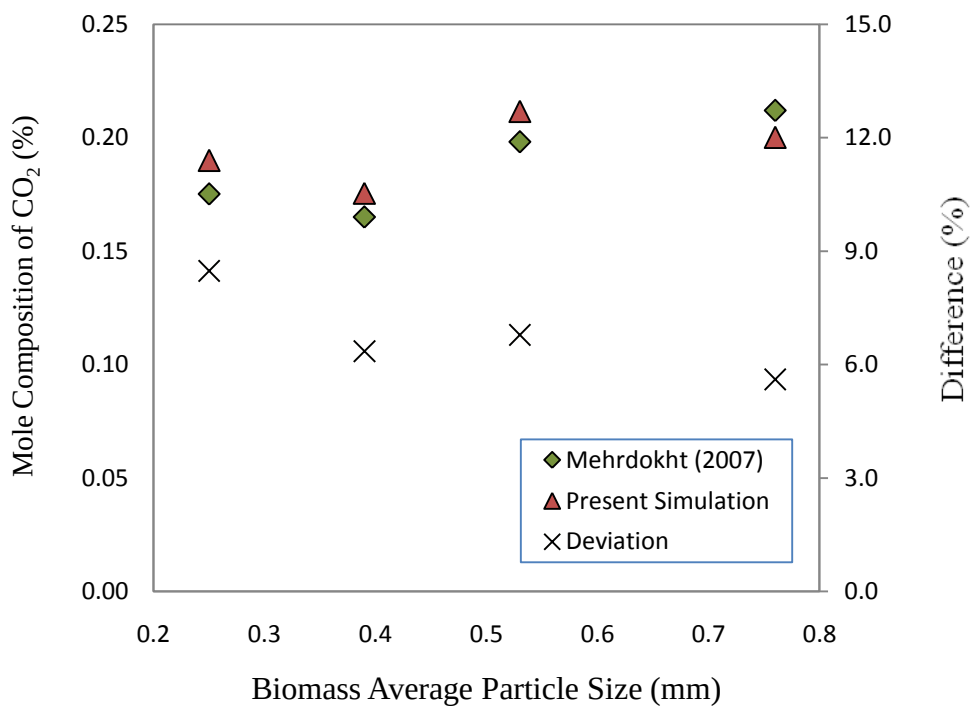


Figure 4.11:Variation of mole composition of CO_2 with biomass particle size and the difference.

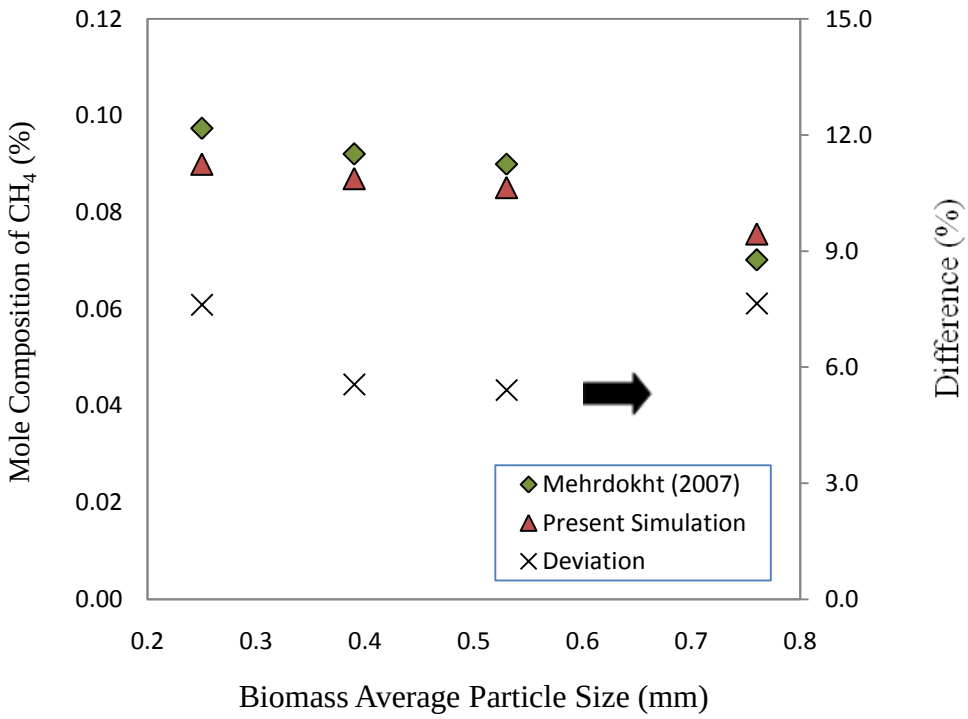


Figure 4.12: Variation of mole composition of CH_4 with biomass particle size and the difference.

4.1.4 Discussion for the Duplication of Past Work Paper

Calculation of Error between Present Simulation and Mehrdokht's Work

1. Sample Calculation for Methane at 700°C

Formula for calculating difference

$$\% \text{ Difference} = \left| \frac{\text{Mehrdokht's Work} - \text{Present Simulation value}}{\text{Mehrdokht's Value}} \right| \text{ x } 100\% \qquad (4.1)$$

$$= \frac{0.09841 - 0.09715}{0.09841} \text{ x } 100\% = 1.28\ \%$$

Note: The other data will follow the same flow of calculation.

Tables 4.1 to 4.3 summarize the percentage error between present simulation and Mehrdokht's work for the effect of temperature, equivalent ratio and biomass particle size to the composition of syngas.

Table 4.1: Percentage error of syngas composition with variation in temperature

Temperature (^{0}C)	**Error for CH_4 (%)**	**Error for CO (%)**	**Error for CO_2 (%)**	**Error for H_2 (%)**
700	1.28	1.79	2.96	0.09
750	2.03	7.22	1.07	4.60
800	0.73	5.00	6.41	2.95
850	6.22	2.36	4.52	1.56
900	6.34	2.41	5.25	0.06

Table 4.2: Percentage error of syngas composition with variation in equivalent ratio

Equivalent Ratio, ER	**Error for CH_4 (%)**	**Error for CO (%)**	**Error for CO_2 (%)**	**Error for H_2 (%)**
0.19	8.80	1.45	4.42	3.61
0.21	2.54	1.06	2.94	6.30
0.23	5.44	4.28	5.76	6.06
0.25	7.05	2.81	4.00	1.97
0.27	7.05	4.49	4.90	1.30

Table 4.3: Percentage error of syngas composition with variation in biomass particle size

Biomass Particle Size, mm	**Error for CH_4 (%)**	**Error for CO (%)**	**Error for CO_2 (%)**	**Error for H_2 (%)**
0.25	7.61	4.89	8.47	0.92
0.39	5.55	4.93	6.35	7.16
0.53	5.41	4.87	6.78	5.94
0.76	7.65	2.16	5.60	2.48

After comparing the results with previous studies, it was found that the smallest value of average percentage error is 0.06% and the largest value of percentage error is 8.80 %. All the errors calculated are below 10%. This proves that, the current work done by the author is reliable. Thus, meaning that the future study which will be done by the author will also be reliable.

CHAPTER 5

RESULT AND DISCUSSION

5.1 PART II: Result For Modelling of Simulation Diagram for Biomass Gasification Process.

A series of simulation diagram for biomass gasification process had been constructed and further improved from time to time to obtained the most reliable simulation diagram.. The operating parameters used are temperature, pressure and air fuel ratio and their effect on syngas composition are presented. The result are shown in Figure 5.1 until 5.12.

5.1.1 Effect of Temperature to Composition of Syngas with biomass feed rate of 0.445 kg/h, air flow rate of 0.5 m^3/h and steam flow rate of 1.2 kg/h.

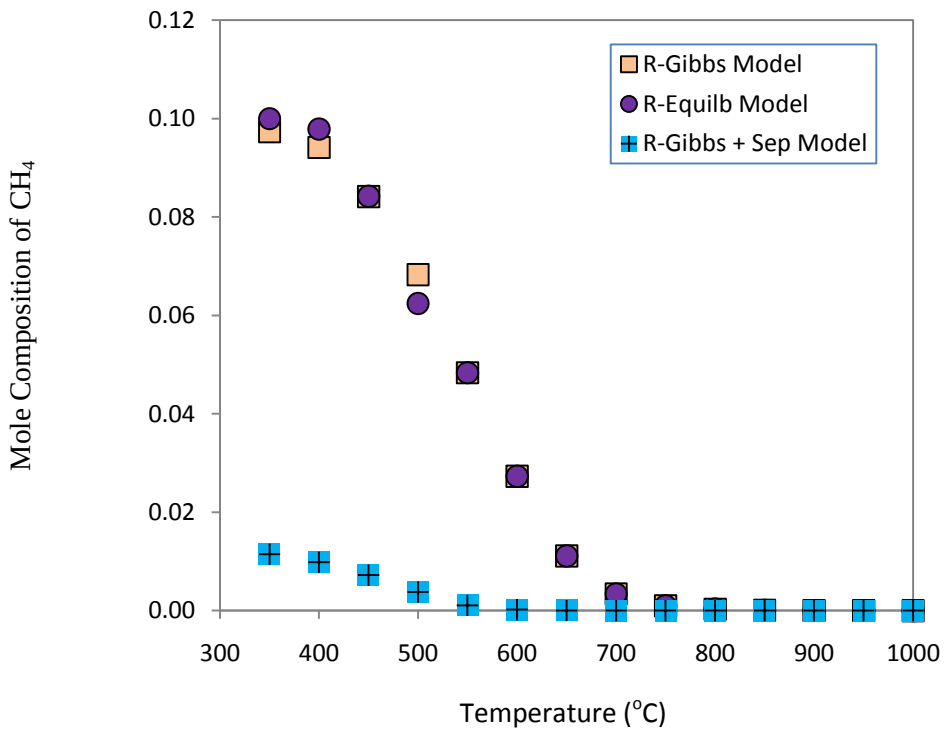


Figure 5.1: Variation of mole composition of CH_4 with temperature for different simulation models.

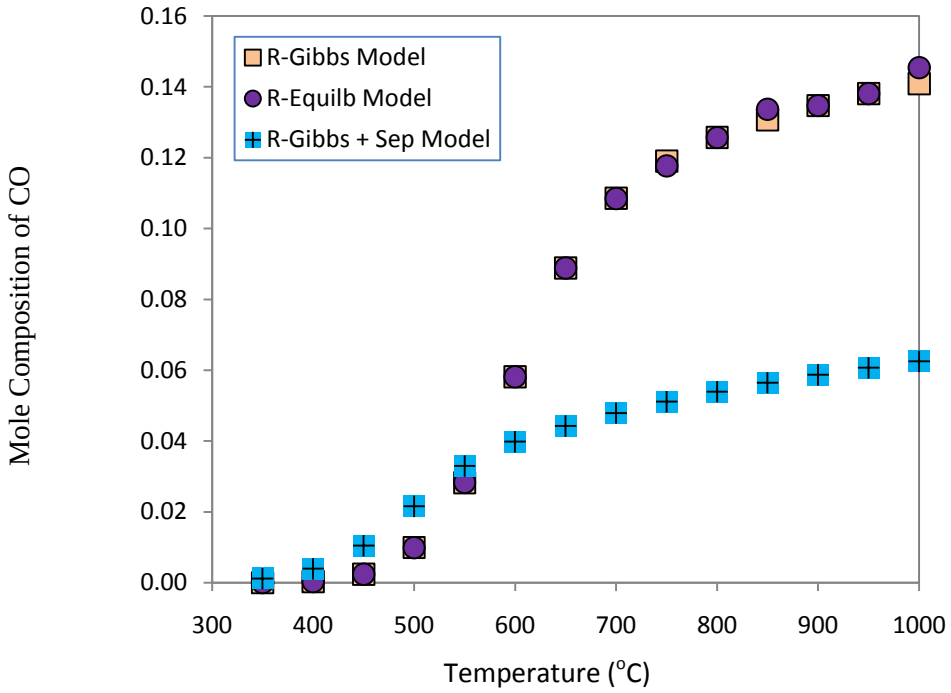


Figure 5.2: Variation of mole composition of CO with temperature for different simulation models.

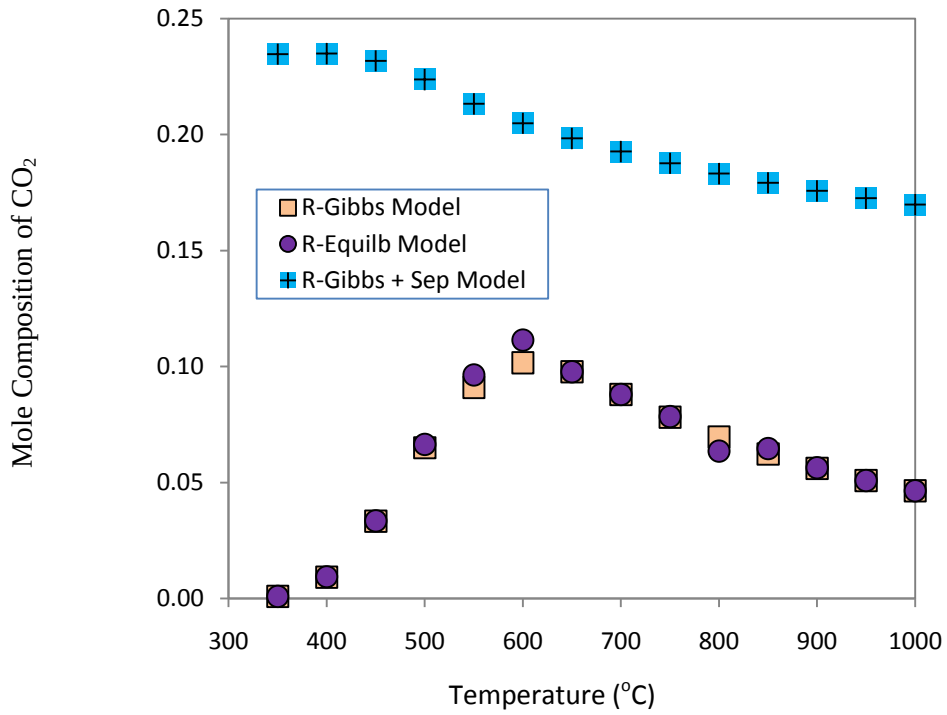


Figure 5.3: Variation of mole composition of CO_2 with temperature at for different simulation models.

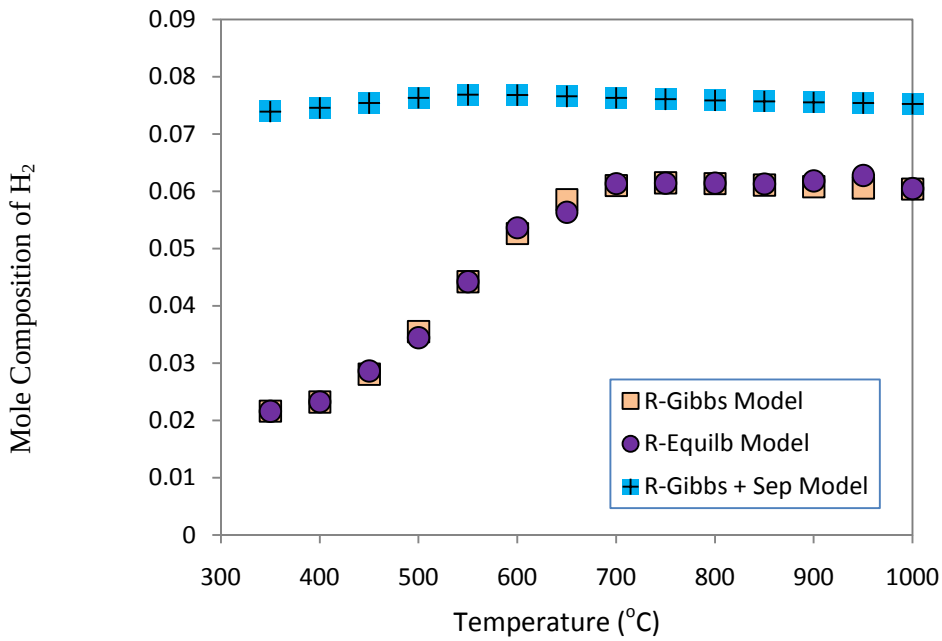


Figure 5.4: Variation of mole composition of H_2 with temperature at for different simulation models.

5.1.2 Effect of Pressure to Composition of Syngas with biomass feed rate of 0.445 kg/h, air flow rate of 0.5 m^3/h and steam flow rate of 1.2 kg/h.

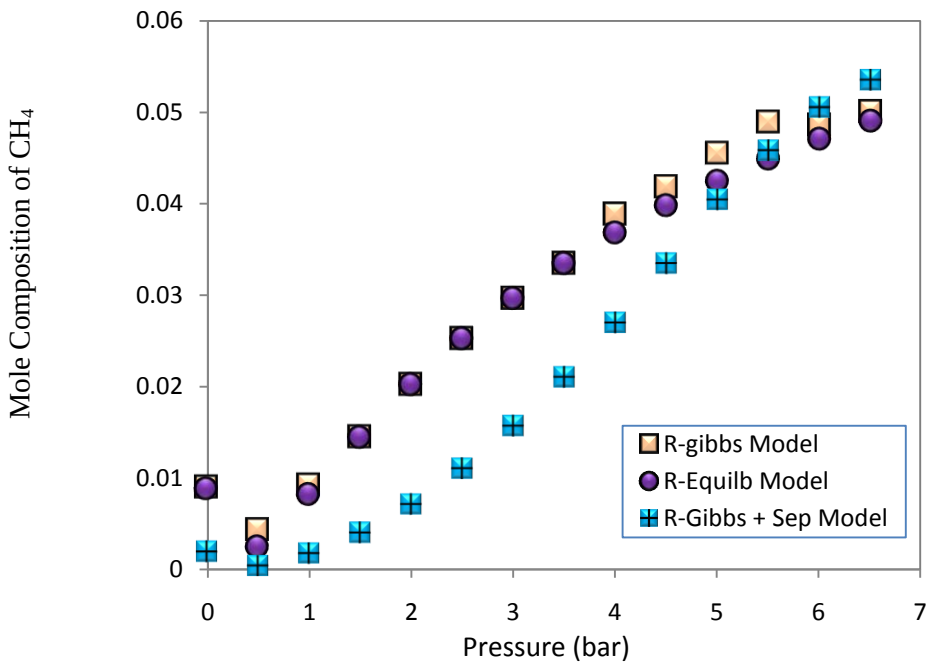


Figure 5.5: Variation of mole composition of CH_4 with pressure for different simulation models.

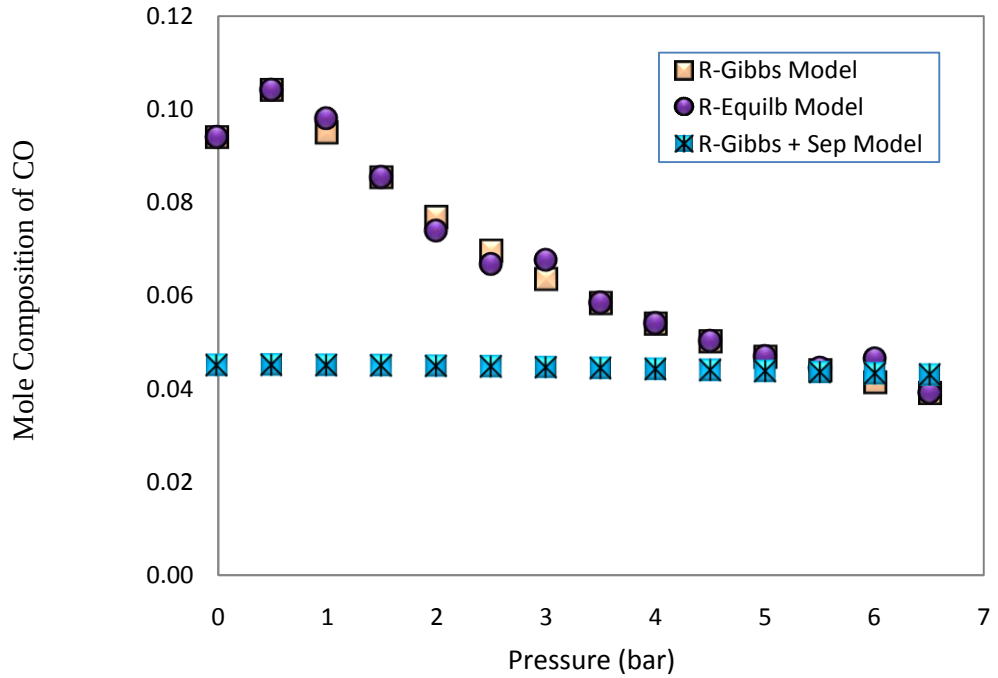


Figure 5.6: Variation of mole composition of CO with pressure for different simulation models.

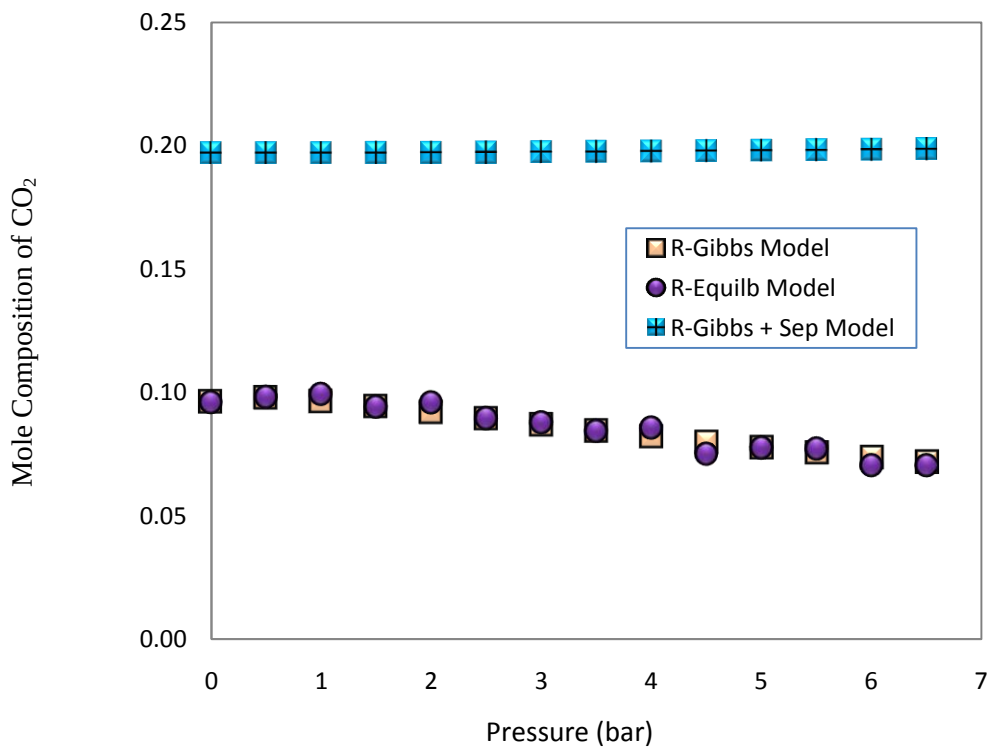


Figure 5.7: Variation of mole composition of CO_2 with pressure for different simulation models.

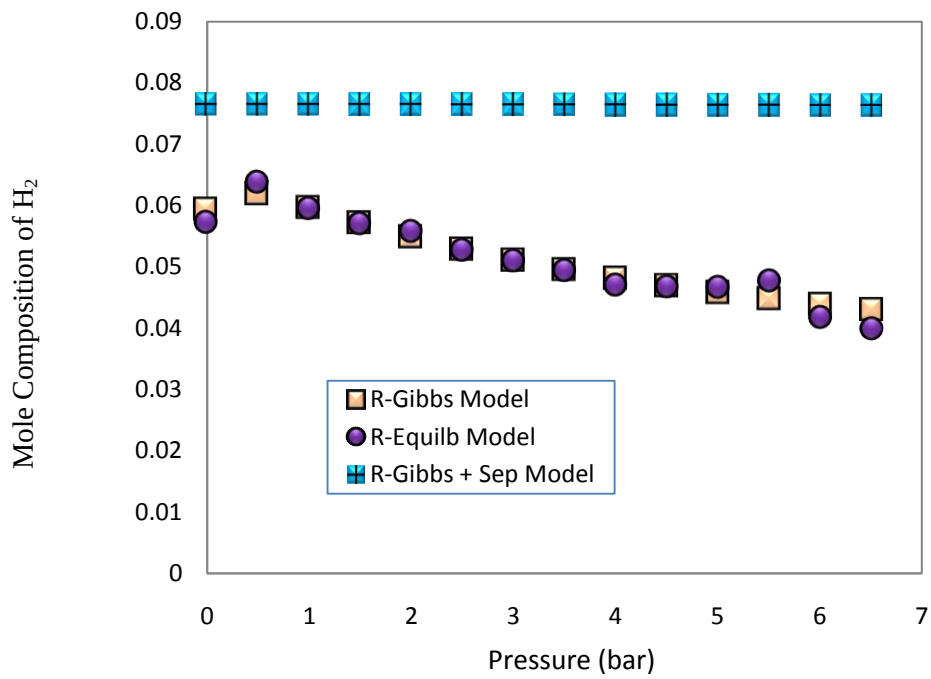


Figure 5.8: Variation of mole composition of H_2 with pressure for different simulation models.

5.1.3 Effect of Air Fuel Ratio, AFR to Composition of Syngas with biomass feed rate of 0.445 kg/h, air flow rate of 0.5 m^3/h and steam flow rate of 1.2 kg/h.

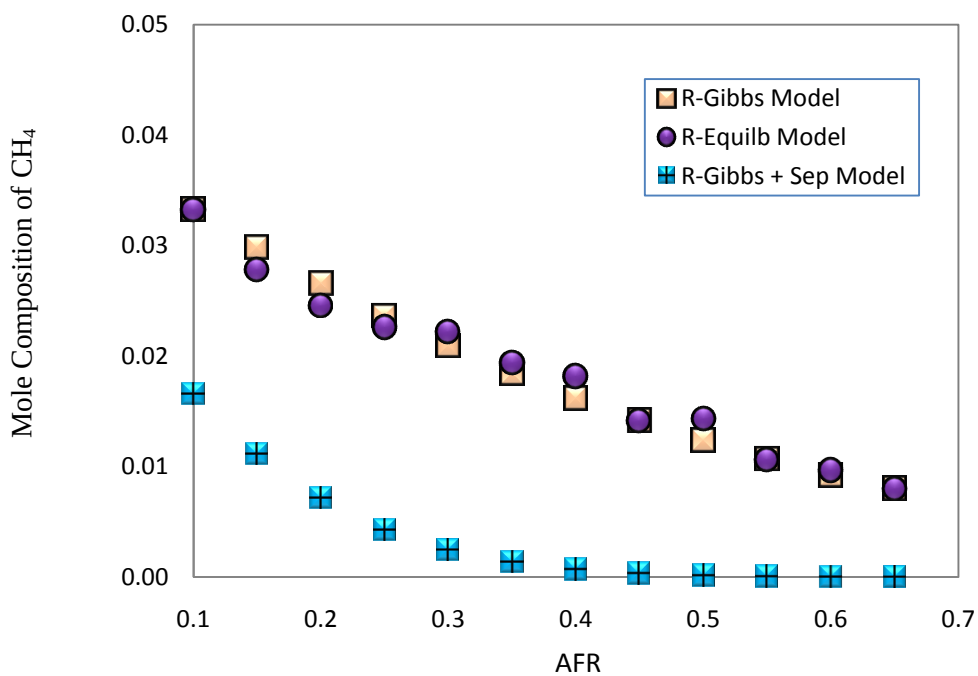


Figure 5.9: Variation of mole composition of CH_4 with AFR for different simulation models.

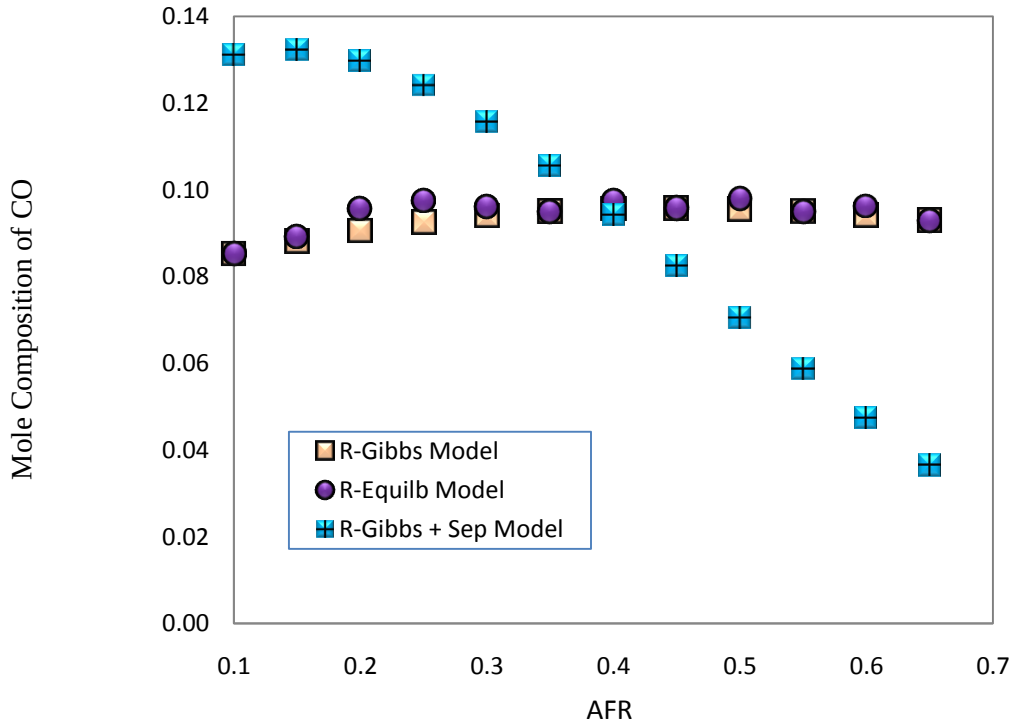


Figure 5.10: Variation of mole composition of CO with AFR for different simulation models.

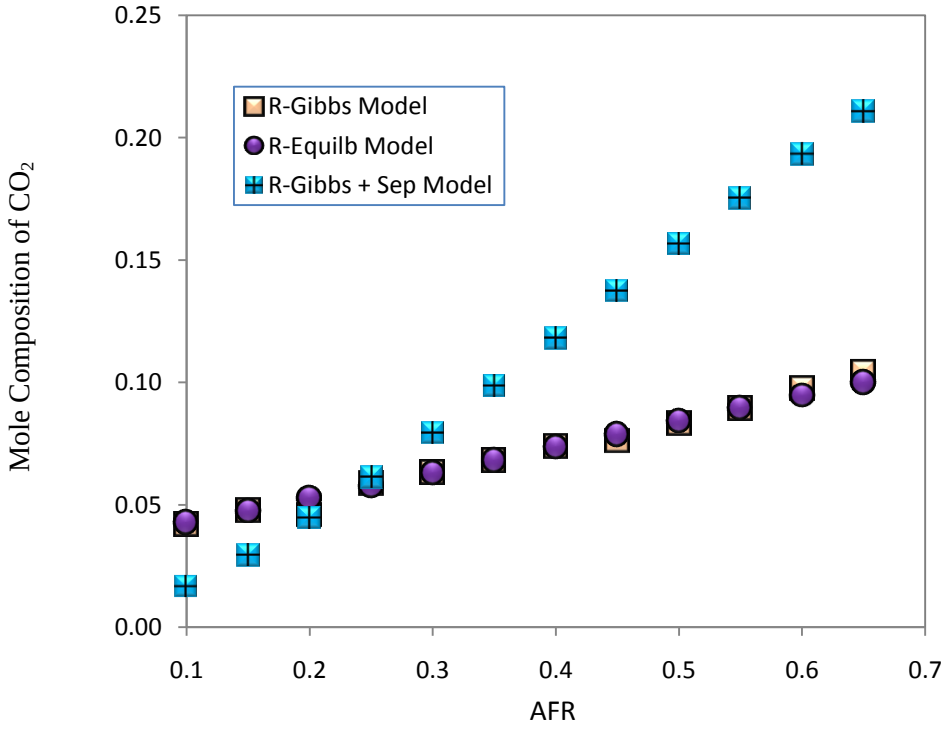


Figure 5.11: Variation of mole composition of CO_2 with AFR for different simulation models

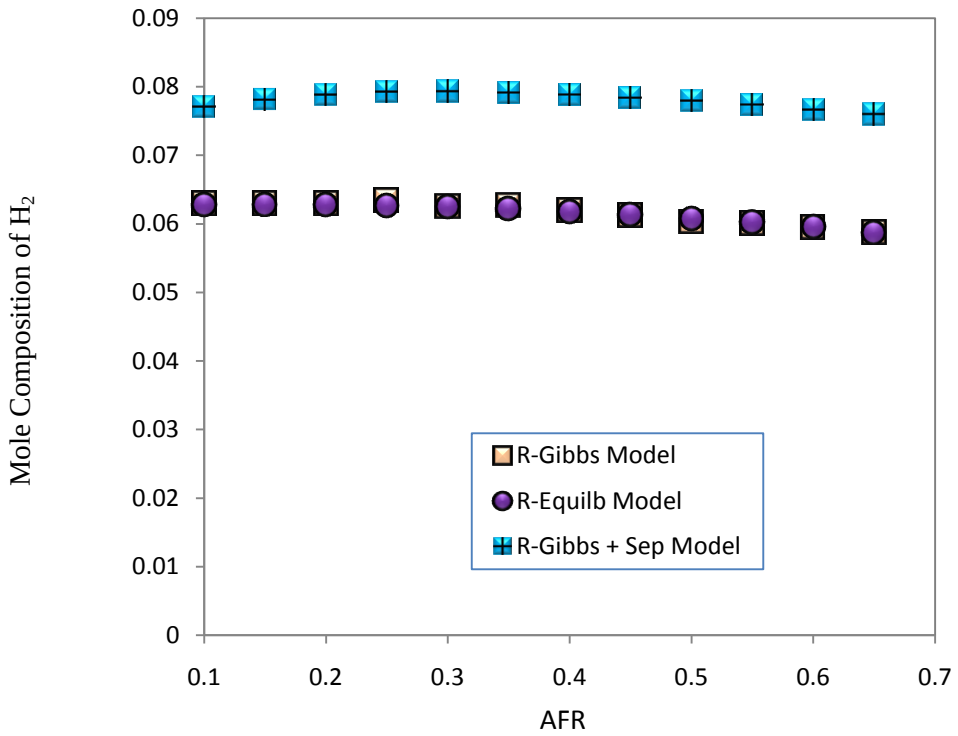


Figure 5.12: Variation of mole composition of H_2 with AFR for different simulation models

5.2 Discussion of Simulation Diagrams for Biomass Gasification Process.

All the three simulation models tend to give a reasonable result. It was clearly seen that the trend and value for R-Gibbs and R-Equilb Model is nearly similar. The different is only that and R-Equilb Model tend to produce a fluctuating result as compare to R-Equilb Model. So, this shows that Gibbs Reactor is a better reactor to be used for biomass gasification process. Basically Gibbs Reactor and Equilibrium Reactor come from the same family that is Equilibrium Based Reactors. The similarities between these two reactor are they do not take reaction kinetics into account, can solve similar problems but problem specifications are different and individual reactions can be at a restricted equilibrium. The differences between these two reactors are as below:

Equilibrium Reactor, R-Equilb.

R-Equilb computes combined chemical and phase equilibrium by solving reaction equilibrium equations. It is useful when there are many components, a few known reactions, and when relatively few components take part in the reactions. But R-Equilb cannot do a 3-phase flash.

Gibbs Reactor, R-Gibbs.

R-Gibbs is the only ASPEN Plus block that will deal with solid-liquid-gas phase equilibrium.

A Gibbs free energy minimization is done to determine the product composition at which the Gibbs free energy of the products is at a minimum. R-Gibbs is quite useful when reactions occurring are not known or are high in number due to many components participating in the reactions.

5.3 Comparison between Simulation Diagrams.

The result form the three simulation diagram is compared with the model form literature. Past work from Kumar et al in 2008 that done a simulation of wood gasification with ASPEN Plus is compared. In their simulation, they use wood as a feedstock and done their simulation using fixed bed gasifier.

5.3.1 Discussion for Temperature

The results for the three simulation diagram on effect of temperature to composition of biomass are shown below. However, the result give by Kumar at el is on mass of biomass versus temperature. Unit conversion is done to make sure the comparison is more reliable based on this formula :

$$m = n \times MW_{OPF} \tag{5.1}$$

where m = Mass of biomass

n = Number of mole

MW = Molecular Weight of OPF ($CH_{1.54}O_{0.88}$) = 27.62

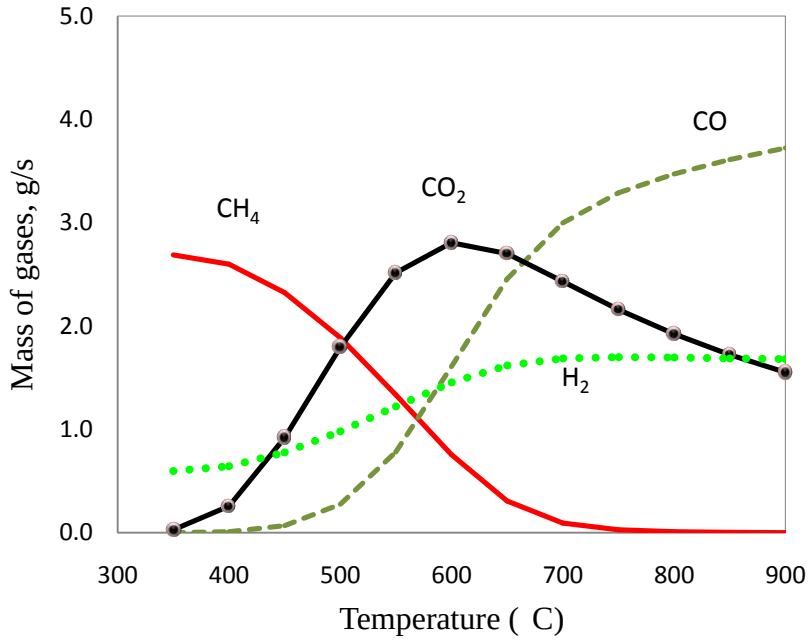


Figure 5.13: Effect of temperature with mass of OPF for R- Gibss Model.

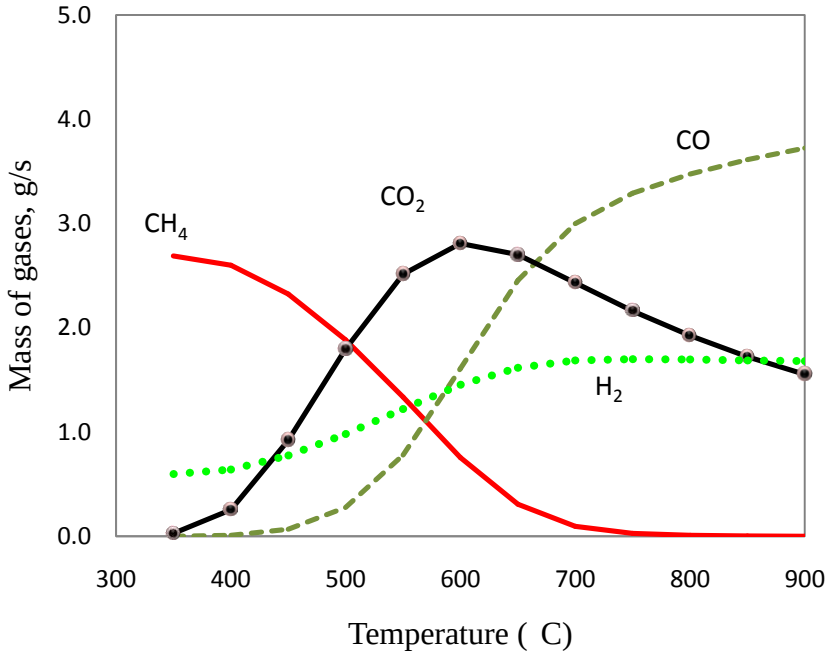


Figure 5.14: Effect of temperature with mass of OPF for R-Equilb Model.

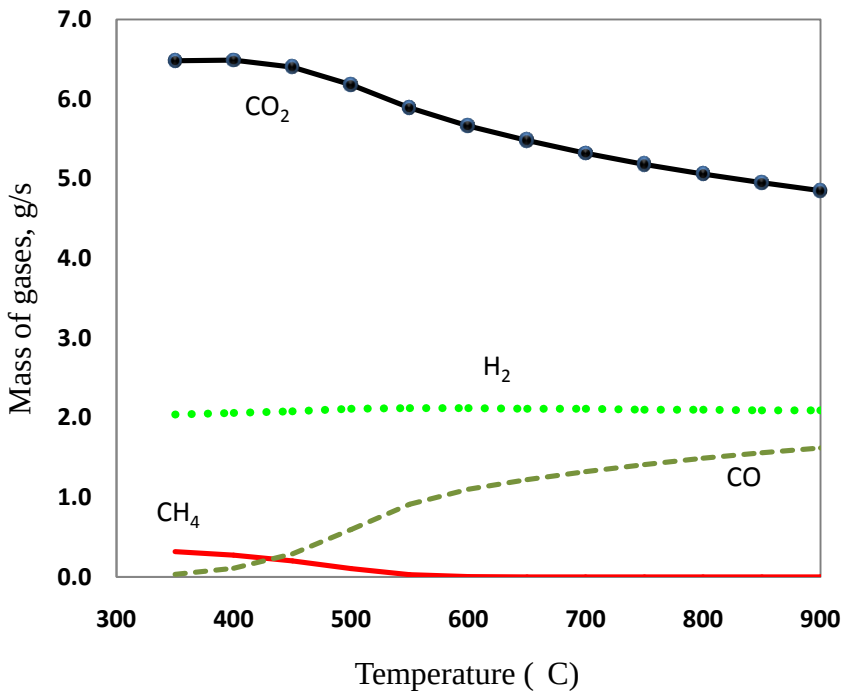


Figure 5.15: Effect of temperature with mass of OPF for R-Gibbs Separator Model

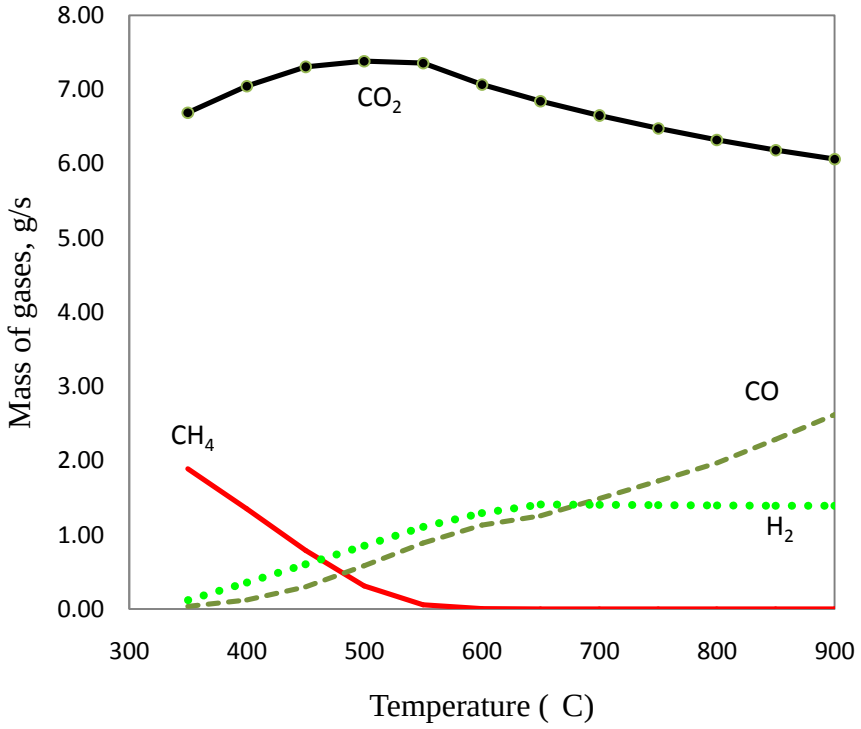


Figure 5.16: Effect of Temperature with composition of syngas. (Kumar et al, 2008): Simulation of wood gasification with ASPEN Plus.

Simulations for the three alternatives were compared with result from Kumar's work. The sum squared deviation method was used to estimate the accuracy of simulation results (Gururajan et al, 1992)

$$\text{RSS} = \sum_{i=1}^{n} \left(\frac{\text{yie} - \text{yip}}{\text{yie}}\right)^2 \tag{5.2}$$

Where yie = experimental value

yip = Present simulation value

$$\text{MRSS} = \frac{\text{RSS}}{\text{N}} \tag{5.3}$$

$$\text{Mean error} = \sqrt{\text{MRSS}} \tag{5.4}$$

The comparison of the result for the three simulations is shown in Table 5.1:

Table 5.1: Comparison between three simulation diagrams for temperature

Simulation Model	**Graph Trend**	**Mean Error**
R-Equilb Model	Slightly Similar	595.293
R-Gibbs Model	Slightly Similar	594.241
R-Gibbs Separator Model	Most Similar	2.329

R-Gibbs Separator Model tends to have the most similar graph trend and the least mean error among the other model when compare with result from Kumar. Production of H_2 is nearly constant over the range of temperature while production of CO_2 is decrease when temperature increases. For production of CO, mole composition is increase when temperature increases. Although it gives the best result at the higher temperature, it is not practical to run an experiment at a very high temperature and safety aspect must also considered. Furthermore, when the experiment runs at high temperature, it required more heat to be used. Based on the result obtained, the best composition of syngas can be estimated to be between 400 – 500 ^{o}C

5.3.2 Discussion for Pressure

Result from past work on variation of pressure with composition of syngas was not available since no past work had done analysis on that. However, based on the graph shown below, it can be said that variation on pressure does not give significant effect to composition of syngas. Below are the graphs of pressure versus mole composition of syngas of the three simulation diagram.

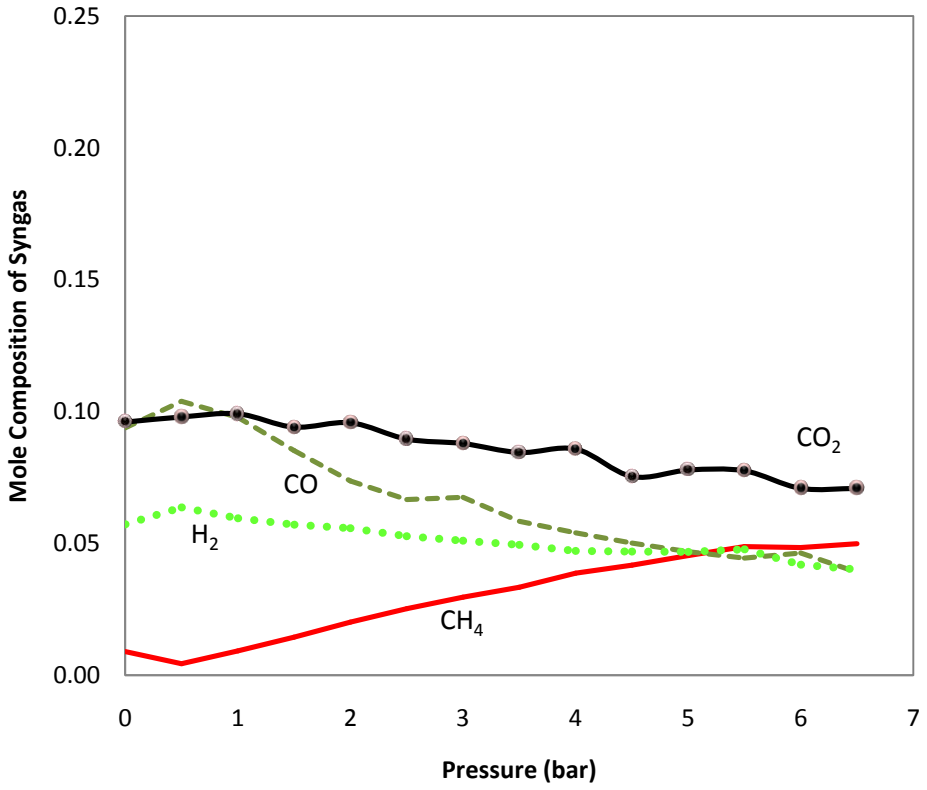


Figure 5.17: Effect of pressure with mass of OPF for R-Equilb Model.

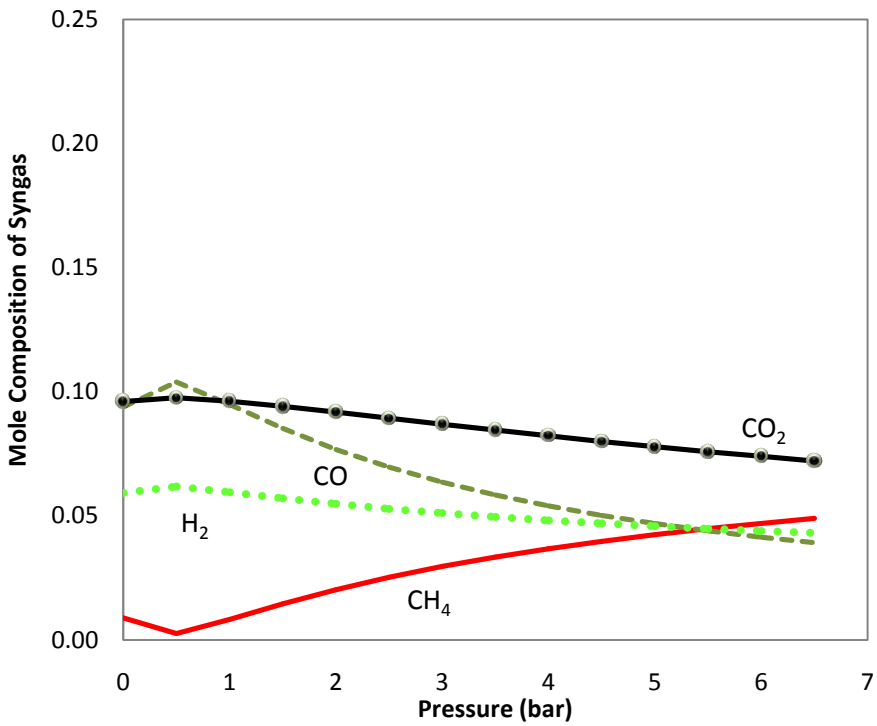


Figure 5.18: Effect of pressure with mass of OPF for R-Gibbs Model.

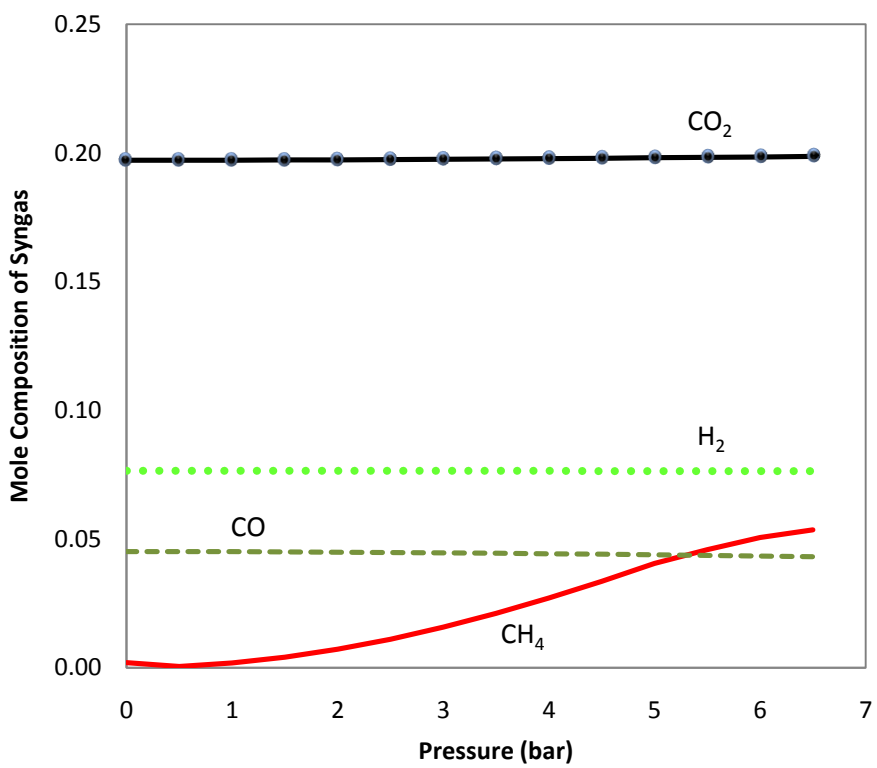


Figure 5.19: Effect of pressure with mass of OPF for R-Gibbs Separator Model.

R-Gibbs Model and R-Equilb Model produce nearly the same result, except that result give by R-Equilb Model tend to produce fluctuating value. Based on these three simulation model, R-Gibbs Separator Model give a more stable and reliable result. For R-Gibbs Separator Model, all the line present tends to give a constant pressure over the range of pressure except for CH_4 that have slightly increase in mole composition at pressure 2 bar and above. In the real situation, the used of high pressure is not practical and small pressure as possible is desired to avoid excessive pressure that has potential to destroy the equipment. So, based on the result obtained, the pressure of 1.0 – 2.0 bar is the optimum pressure that result in the best composition of syngas. To make thing easier, the pressure of 1.01 bar or equal to 1 atm is the practical value to be used.

5.3.3 Discussion for Air Fuel Ratio, AFR

Productions of CO and CH_4 decrease with increase in AFR, while production of CO_2 increases with increase in AFR. Production of H_2 is nearly constant over the range of AFR. R-Gibbs Separator Model is selected based on the comparison with the work form Kumar. Below is the graph of work from Kumar's Work and the three simulation diagram.

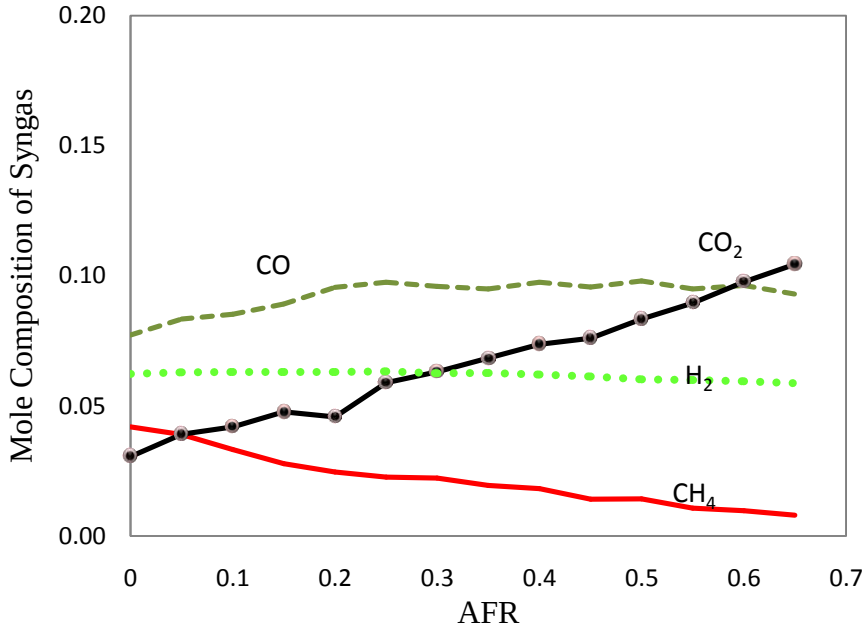


Figure 5.20: Effect of AFR with mass of OPF for R-Equilb Model.

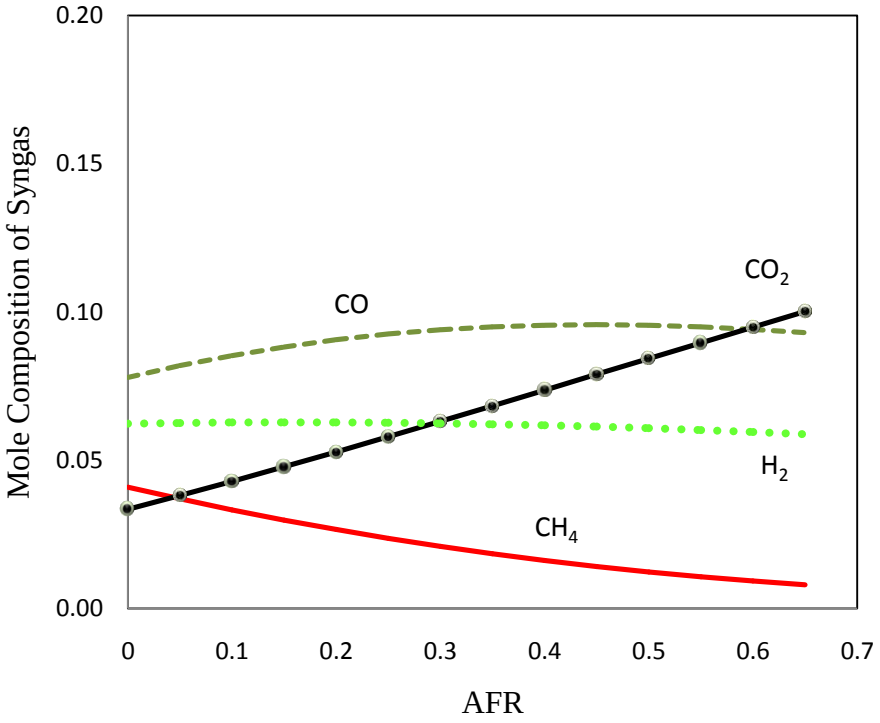


Figure 5.21: Effect of AFR with mass of OPF for R-Gibbs Model.

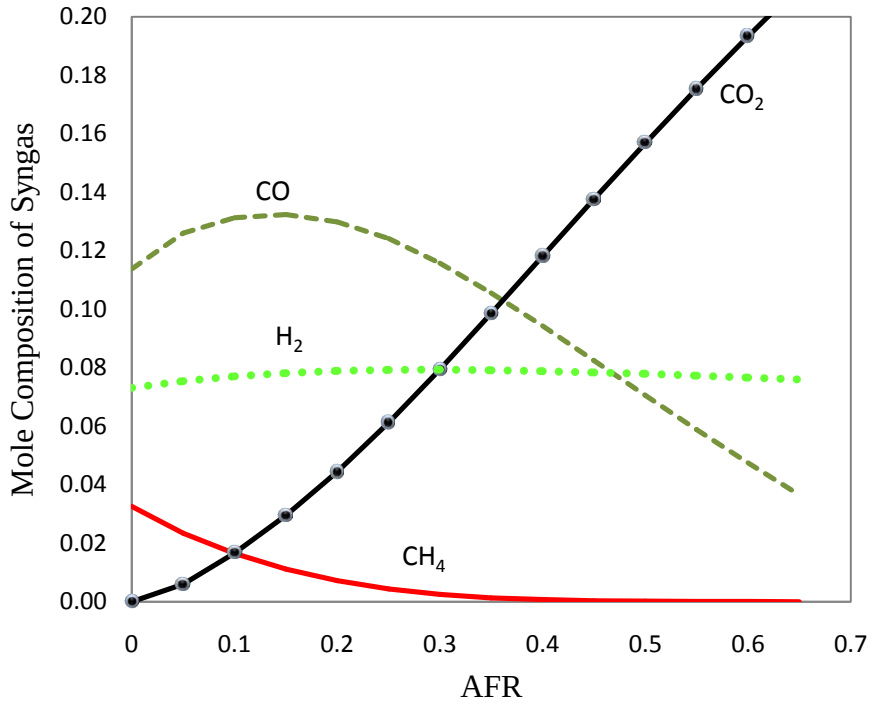


Figure 5.22: Effect of AFR with mass of OPF for R-Gibbs Separator Model.

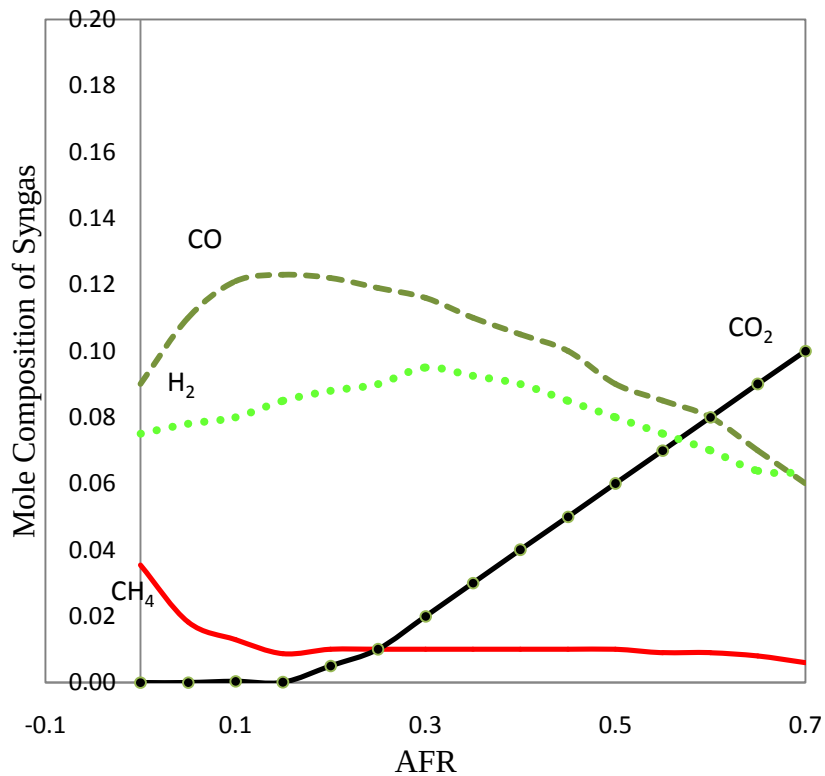


Figure 5.23: Effect of Air Fuel Ratio with mole composition of syngas. (Kumar et al, 2008): Simulation of wood gasification with ASPEN Plus.

Some calculation of percentage error of the three simulation diagram with respect to work by Kumar is done. The result is shown in Table 5.2.

Table 5.2: Comparison between three simulation diagrams for air fuel ratio

Simulation Model	Graph Trend	Mean Error
R-Equilb Model	Slightly Similar	966.4
R-Gibbs Model	Slightly Similar	922.2
R-Gibbs Separator Model	Most Similar	83.6

Note: Formula for calculating difference is same as before for temperature.

R-Gibbs Separator Model tends to have the most similar graph trend and the least mean error among the other model when compare with result from Kumar. CO_2 increases with increasing AFR while H_2 maintain its production over range value of AFR. CH_4 tends to

give reasonable output at AFR less than 0.3 while CO give maximum output at AFR approximately 0.1 – 0.2. Based on the result obtained from the four components of syngas, AFR of 0.1 - 0.2 is the optimum value that results in the best composition of syngas.

In Summary, the selection of the R-Gibbs Separator Model as the best model is not means that the other two simulation diagram is wrong.n But it is choose based on the comparison with literature. Although the feedstock is not the same, wood and oil palm frond can be predicted to have nearly same characteristic. The install separator tends to increase the accuracy of the result since it removes all the impurities before the dried OPF being combusted and reduced. The final product will nearly free from tar and give an accurate result. It is best to compare this project with experimental work. So for further recommendation, hopefully someone can do the real experiment of this project.

CHAPTER 6

CONCLUSIONS AND RECOMMENDATIONS

6.1 Conclusions

The project has successfully met all its predetermined objectives with the main goal is to determine the optimum operating conditions that would result in the best composition of syngas by means of ASPEN Plus software. Downdraft type gasifier provides a low tar content and is designed based on Imbert gasifier principle. ASPEN Simulator Software is a very suitable tool to develop a model of gasification process. A model for gasification of biomass in fluidized bed gasifier using the ASPEN Plus software was successfully replicated that shows that the author's work is reliable.

Model of gasification process in downdraft gasifier using OPF as a feedstock had successfully design in which the best simulation diagram is chosen based on the comparison from past work. The simulation results for the product gas composition versus temperature, pressure steam-to-biomass ratio, and air fuel ratio were obtained.

The optimum operating condition had successfully determined in this project.

1. Temperature range of 400 – 500°C
2. Air fuel ratio range of 0.1 – 0.2
3. Pressure range of 1.0 – 2.0 bar

6.2 Recommendations

To achieve a better result, some modification can be made. In the present simulation Mass transfer inside solid particles and heat transfer inside particles is not considered. Mass transfer inside solid particles is an important parameter in gas–solid reactions, and heat transfer inside particles, between phases, and between material and wall is feature that should be included in order to achieve better simulation prediction.

The selection of the best simulation model is based on the comparison made between the present simulation and pass work. But, the pass work paper use wood as feedstock. To gain a better agreement of the result, an experiment that used OPF as feedstock should be made and compare the result with the present simulation.

It is hoped that the present research would provide a platform for future application of the project on large scale. A successful application of the present work on a large scale system would provide as an alternative way to reduce the dependent on non-renewable energy.

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APPENDICES

Effect of Temperature on Composition of Syngas.

i.Data from past Mehrdokht's work

Table A-1 : Effect of temperature on composition of syngas from Mehrdokht's work

Temperature (^{0}C)	Mole of CH4, mol	Mole of CO, mol	Mole of CO2, mol	Mole of H2, mol
700	0.09841	0.46584	0.22005	0.30142
750	0.08151	0.43247	0.21124	0.33674
800	0.07854	0.40441	0.20214	0.36076
850	0.06945	0.37165	0.20114	0.37802
900	0.06514	0.34411	0.20001	0.39959

ii.Data from present simulation

Table A-2 : Effect of temperature on composition of syngas from present simulation

Temperature (^{0}C)	Mole of CH4, mol	Mole of CO, mol	Mole of CO2, mol	Mole of H2, mol
700	0.09715	0.47422	0.21352	0.30112
750	0.08317	0.40124	0.21352	0.32124
800	0.07912	0.42464	0.21511	0.37142
850	0.06013	0.38045	0.21024	0.37211
900	0.06101	0.35243	0.21052	0.39985

Effect of Equivalent Ratio on Composition of Syngas.

i.Data from Mehrdokht's work

Table A-3 : Effect of equivalent ratio on composition of syngas from Mehrdokht's work

Equivalent Ratio, ER	Mole of CH4, mol	Mole of CO, mol	Mole of CO2, mol	Mole of H2, mol
0.19	0.08154	0.39541	0.20111	0.32154
0.21	0.09144	0.41568	0.18412	0.30245
0.23	0.07511	0.42158	0.16841	0.31115
0.25	0.08421	0.39999	0.20145	0.30111
0.27	6.12E-02	0.37145	0.22159	0.31541

ii.Data from present simulation

Table A-4 : Effect of equivalent ratio on composition of syngas from present simulation

Equivalent Ratio, ER	Mole of CH4, mol	Mole of CO, mol	Mole of CO2, mol	Mole of H2, mol
0.19	0.08872	0.40115	0.19221	0.33315
0.21	0.08911	0.42011	0.18954	0.32153
0.23	0.07102	0.43965	0.17812	0.33002
0.25	0.09015	0.41121	0.20951	0.29516
0.27	6.56E-02	0.38814	0.23245	0.31954

Effect of Biomass Particle Size (BPS) on Composition of Syngas.

i.Data from Mehrdokht's work

Table A-5 : Effect of BPS on composition of syngas from Mehrdokht's work

Biomass Particle Size, mm	Mole of CH4, mol	Mole of CO, mol	Mole of CO2, mol	Mole of H2, mol
0.25	0.09741	0.42151	0.17514	0.32412
0.39	0.09211	0.40541	0.16504	0.33513
0.53	0.09001	0.38141	0.19811	0.34922
0.76	0.07018	0.37015	0.21201	0.35121

ii.Data from present simulation

TableA-.6 : Effect of BPS on composition of syngas from present simulation

Biomass Particle Size, mm	Mole of CH4, mol	Mole of CO, mol	Mole of CO2, mol	Mole of H2, mol
0.25	0.09715	0.47422	0.21352	0.30112
0.39	0.08317	0.40124	0.21352	0.32124
0.53	0.07912	0.42464	0.21511	0.37142
0.76	0.06013	0.38045	0.21024	0.37211

Input Summary created by ASPEN Plus Rel. 21.0 at 00:25:25 Fri Apr 09, 2010

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TITLE ' FYP project redzuan computer simulation of biomass gasification process'

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      HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=C  &
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   C, bar, kg/hr, kmol/hr, Gcal/hr, cum/hr.

   Property Method: None

   Flow basis for input: Mole

   Stream report composition: Mole flow
   "

DATABANKS PURE20  / AQUEOUS  / SOLIDS  / INORGANIC  /  &
      NOASPENPCD

PROP-SOURCES PURE20  / AQUEOUS  / SOLIDS  / INORGANIC

COMPONENTS
```

```
   H2 H2 /
   O2 O2 /
   CO CO /
   CO2 CO2 /
   H2O H2O /
   N2 N2 /
   CH4 CH4 /
   S S /
   C C /
   BIOMASS /
   ASH

FLOWSHEET
   BLOCK RYIELD IN=FEED OUT=S1
   BLOCK R-GIBBS IN=S1 OUT=S4
   BLOCK MIXER IN=S4 AIR STEAM OUT=S5

PROPERTIES IDEAL

NC-COMPS BIOMASS PROXANAL ULTANAL SULFANAL

NC-PROPS BIOMASS ENTHALPY HCOALGEN / DENSITY DCOALIGT

NC-COMPS ASH PROXANAL ULTANAL SULFANAL

NC-PROPS ASH ENTHALPY HCOALGEN / DENSITY DCOALIGT

STREAM AIR
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   MOLE-FRAC O2 0.21 / N2 0.79
```

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   MASS-FRAC BIOMASS 1.
   COMP-ATTR BIOMASS PROXANAL ( 4. 39.7 51.3 6.3 )
   COMP-ATTR BIOMASS ULTANAL ( 0.55 42.55 5.48 2.18 0.  &
      0.11 41.11 )
   COMP-ATTR BIOMASS SULFANAL ( 0.57 0. 0. )
   SUBS-ATTR PSD ( 0. 1. 0. 0. )

STREAM STEAM
   SUBSTREAM MIXED TEMP=154. PRES=1.05 MASS-FLOW=0.8
   MASS-FRAC H2O 1.

BLOCK MIXER MIXER

BLOCK RYIELD RYIELD
   PARAM TEMP=25. PRES=1.05
   MASS-YIELD MIXED H2O 0.1 / C 0.1 / H2 0.1 / O2 0.1 /  &
      N2 0.1 / S 0.1 / NCPSD ASH 0.1
   COMP-ATTR NCPSD ASH PROXANAL ( 0. 0. 0. 100. )
   COMP-ATTR NCPSD ASH ULTANAL ( 100. 0. 0. 0. 0. 0. 0.  &
      )
   COMP-ATTR NCPSD ASH SULFANAL ( 0. 0. 0. )
   SUBS-ATTR 1 CIPSD PSD ( 0. 1. 0. 0. )
   SUBS-ATTR 2 NCPSD PSD ( 0. 1. 0. 0. )

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   PARAM TEMP=660. PRES=1.05
   PROD CH4 / H2 / O2 / CO / CO2 / H2O / N2 / S

EO-CONV-OPTI
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      SENTENCE=PARAM
   DEFINE PRES BLOCK-VAR BLOCK=RYIELD VARIABLE=PRES  &
      SENTENCE=PARAM
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      VARIABLE=MASS-FLOW
   DEFINE CO2 STREAM-VAR STREAM=S5 SUBSTREAM=MIXED  &
      VARIABLE=MASS-FLOW
   DEFINE H2 STREAM-VAR STREAM=S5 SUBSTREAM=MIXED  &
      VARIABLE=MASS-FLOW
   DEFINE CO STREAM-VAR STREAM=S5 SUBSTREAM=MIXED  &
      VARIABLE=MASS-FLOW
   DEFINE S1 STREAM-VAR STREAM=S1 SUBSTREAM=MIXED  &
      VARIABLE=MASS-FLOW
   DEFINE S4 MASS-FLOW STREAM=S4 SUBSTREAM=MIXED COMPONENT=CO2
   DEFINE S5 MASS-FLOW STREAM=S5 SUBSTREAM=MIXED COMPONENT=CH4
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   TABULATE 2 "S5"
   VARY BLOCK-VAR BLOCK=RYIELD VARIABLE=PRES SENTENCE=PARAM
   RANGE LOWER="0.5" UPPER="10.5" INCR="1"
;
;
;
;
;
```