

Simulation of Gasification of Empty Fruit Bunches to Produce Hydrogen

by

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the requirements for the
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CERTIFICATION OF APPROVAL

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A project dissertation submitted to the
Chemical Engineering Programme
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Approved by,



(Dr. Murni Melati bt. Ahmad)

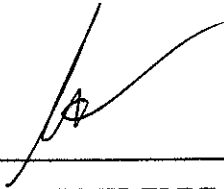
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January 2009

CERTIFICATION OF ORIGINALITY

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the references and acknowledgements, and that the original work contained herein have not been undertaken or done by unspecified sources or persons.



MUHAMMAD TARMIDZI BIN SAMSUDIN

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CHAPTER 1

1. INTRODUCTION

1.1 Overview

The world is facing a crucial situation nowadays in which the fossil fuel reservoir is depleting while the demand for energy is increasing worldwide. Scientists around the world have shifted their attention towards developing alternative sustainable fuels and quite a number of technologies have been discovered; say the production of energy from the electrolysis of water. The technology itself has attracted many researchers but the problem faced with the technology is the high cost required to produce the fuel cell. Another potential alternative solution that has also attracted many researchers is to produce energy from hydrogen via chemical reaction. Hydrogen is the most abundant element on earth. One of the methods to produce hydrogen is through the natural gas reforming process. However, this method is not favorable for long term implementation and large scale hydrogen production since the natural gas itself is not a sustainable resource. Another potential method to produce hydrogen is via thermal conversion of biomass. The aforementioned process can be divided into 2 distinct processes which are the pyrolysis process and the gasification process. The differences between these 2 processes are the reaction path they undergo in order to produce hydrogen. For the pyrolysis process, the biomass is first converted to bio-oil before producing hydrogen. On the other hand, the gasification process directly converts the biomass to hydrogen.

1.2 Gasification Process

In this work, the hydrogen production method that is selected for feasibility studies is the gasification process. Gasification is simply the conversion of biomass to a gaseous fuel by heating in a gasification medium such as air, oxygen or steam. The process converts the intrinsic chemical energy of the carbon in the biomass into combustible gases.

The energy efficiency in the case of gasification is higher than that of combustion. Though, one of the disadvantages of gasification is how to deal with the tar formed in the process. The quality of the gas produced can be standardized, easier and more versatile to use compared to the original biomass. The gas can be used to power gas engines and gas turbines. The gas can also be used as a chemical feedstock to produce liquid fuels.

A typical gasification process takes place at high temperature (1500°F), in an atmosphere of steam or air (or both), with approximately 30% the amount of oxygen needed for ideal combustion [2]. The mixture of gases produced is about one third hydrogen. Removing the hydrogen and subjecting the other gases and materials to high temperature steam produces a synthesis gas, or “syngas” (composed of carbon monoxide and hydrogen). The water shift reaction converts carbon monoxide and steam into more hydrogen. The emissions from biomass combustion systems, including the products of complete combustion (CO_2) and incomplete combustion (CO, char particles, tar, polycyclic aromatic hydrocarbons and other organic compounds), as well as NO_x , SO_2 , HCl and ash particles, are affected by the combustion method as well as by the operating conditions and fuel properties.

1.3 Types of Gasification Methods

There are several types of gasification methods which employs different combination of gasification medium. Different types of gasification medium would produce different product gas compositions and would also affect the energy content of the product gas. The low calorific value (CV) gas can be used directly for the engine

fuel, while the medium and high CV gas can be utilized as feedstock for subsequent conversion into basic chemicals such as methane and methanol [10].

Table 1: Classification of gasification [3]

Gasification Methods	Product Gas Energy Content	Product Gas
Steam + Air	Low BTU gas	CO, H ₂ , N ₂
Steam + O ₂	Medium BTU gas	CO, H ₂
Steam + Heat	Medium BTU gas	CO, H ₂
Hydrogen + Heat (Hydrogasification)	High BTU gas	CO, H ₂ , CH ₄
Steam (Catalytic gasification)	SNG (Substitute Natural Gas)	CH ₄

1.4 Types of Gasifier

There are 2 main types of gasifier that is commonly used in the industry which are;

- a) **Fixed bed gasifier:** Fixed bed gasifiers have the advantage of a simple design but the disadvantage of producing a low CV gas with high tar content. Improvements to gas quality have been proposed by operating a two-stage, two reactor processes. Pyrolysis of the biomass takes place in the first stage using external heating at 600°C. The gases formed in the first stage are then reacted with steam to crack the tars. In the second stage the gases react with the char from the first stage to produce the final product gas. Fixed bed gasifiers generally produce a lower particulate load than a fluidized bed gasifier. Research has shown the fixed bed, downdraft gasifier to be most capable of producing a low tar content / tar-free gas.

- i. **Updraft** (Feed introduced at the top and air at the bottom)

Due to the low temperature of the gas leaving the gasifier, the overall energy efficiency of the process is high but so also is the tar content of the gas.

ii. Downdraft

Because the gases leave the gasifier unit at temperatures about 900-1000°C, the overall energy efficiency of a downdraft gasifier is low, due to the high heat content carried over by the hot gas. The tar content of the product gas is lower than for an updraft gasifier but the particulates content of the gas is high.

iii. Cross-flow

Ash is removed at the bottom and the temperature of the gas leaving the unit is about 800-900°C: as a consequence this gives low overall energy efficiency for the process and a gas with high tar content.

b) **Fluidized bed gasifier:** Its advantage over fixed bed gasifiers is the uniform distribution of temperature in the gasification zone. The major operational difficulty is slagging of the bed material due to the ash content in the biomass. The required degree of clean-up can be achieved by either hot or cold gas cleaning. Hot gas cleaning is much more technically challenging compared to cold gas cleaning.

i. Circulating fluidized bed

It is able to cope with high capacity throughputs. The gasifier can also be operated at elevated pressures.

ii. Bubbling bed

The product gas has low tar content, typically $< 1-3 \text{ g/Nm}^3$.

1.5 Empty Fruit Bunch (EFB)

In this work, the source of hydrogen is from the gasification of empty fruit bunch of the palm oil. In many countries, wood supply (as fuel) can no longer meet the demand and very few countries have excess wood for gasification or charcoal production without serious impact on their natural resources. The feasibility of this project lies on the fact that there are more than 3 million hectares of oil palm plantations in Malaysia and each year, about 90 million metric ton of renewable biomass (trunks, fronds, shells, palm press fiber and the EFB) are produced. The EFB are the residue left after the fruit bunches are pressed at oil mills, and the oil extracted. The EFB represent about 9% of the total renewable biomass. It is estimated that about 6.67 million metric ton per year of EFB are produced in Malaysia in 2006 and from that amount of EFB produced, Malaysia is able to produce 3.33 million metric ton hydrogen per year and satisfies 8% of the world demand [11].

1.6 Problem Statements

Hydrogen can be converted to heat and power through chemical reactions. But nature does not provide hydrogen in its elemental form. Electricity or heat is needed to liberate hydrogen from its chemical source. One of the chemical sources that are being used to synthesize hydrogen is the natural gas. Hydrogen can be produced from methane through steam methane reforming. But there is a limited supply of natural gas so large-scale production of hydrogen is not considered a long-term option. Other promising alternatives to produce hydrogen are through pyrolysis and gasification of biomass; in this case the EFB. It is currently concluded that pyrolysis has several advantages over gasification such as better transportability and potential production and recovery of higher value added co-products from bio-oil [4]. It is of interest to investigate up to which extent that the gasification process economically feasible and also the technically optimal. For those purposes, the modeling and simulation approach is implemented due to the exhaustive range of operating conditions and it will be less expensive rather than directly executing the process at plant scale or even lab scale.

1.7 Objectives

The objectives of this work include;

- a) To screen process alternatives to produce hydrogen from EFB.
- b) To synthesize and develop the process to produce hydrogen from EFB.
- c) To perform simulations for the developed flowsheet in iCON.
- d) To study the technical and economical feasibility of gasification process of EFB into hydrogen at industrial scale, via the simulation.
- e) To determine the optimum operating conditions for the production of hydrogen from the EFB.

1.8 Scope of Study

The gasification process will be taken into consideration for the thermal conversion of biomass. Typical sources of biomass that is used to produce hydrogen include fibre, starches and sugars from trees, woody plants and crops, and food processing residues but for the purpose of this research the source of biomass is taken as the EFB from the oil palm waste because of the fact that Malaysia is the largest palm oil producer in the world and has abundant resources of the EFB produced each year. The gasification method that will be considered in this work is the oxygen-steam gasification integrated with the adsorption of carbon dioxide using calcium oxide with the operating conditions between 600-1000°C. The gasification of the EFB will be simulated in a bubbling fluidized bed gasifier using the iCON software. Before any simulations can take place, various data such as the properties of the EFB, the initial operating conditions of the gasification process and the estimated yield of hydrogen gas has to be pre-determined. Those data are obtained from established literature reviews. The summary of the literature researches will be discussed in the next chapter.

CHAPTER 2

2. LITERATURE REVIEW

2.1 Modelings and Simulations of Biomass Gasification

Laihong Shen, Yang Gao and Jun Xiao had reported in their work entitled, **“Simulation of hydrogen production from biomass gasification in interconnected fluidized beds”** [8] that at gasifier temperature of 750-800°C and with steam-to-biomass ratio of 0.6-0.7, the hydrogen yield ranged from 54-63g H₂ per kg biomass. The gasification process was simulated using ASPEN PLUS in an interconnected fluidized bed reactor system with steam as the gasification medium.

The following assumptions were made based on the application of ASPEN PLUS software;

- a) The combustor and the gasifier were operated under steady state.
- b) Ash in the biomass as well as in bed particles (sand) was inert.
- c) Tar was not taken into account in the simulation.

The operating conditions and primary parameters in the simulations were;

Table 2: Operating conditions of the gasification process

Biomass flow rate	1 kg/s
Air flow rate	2 kg/s
Steam temperature	600°C
H ₂ -rich gas	500°C
Combustor temperature	920°C
Gasifier temperature	650-900°C
System pressure	0.1 MPa

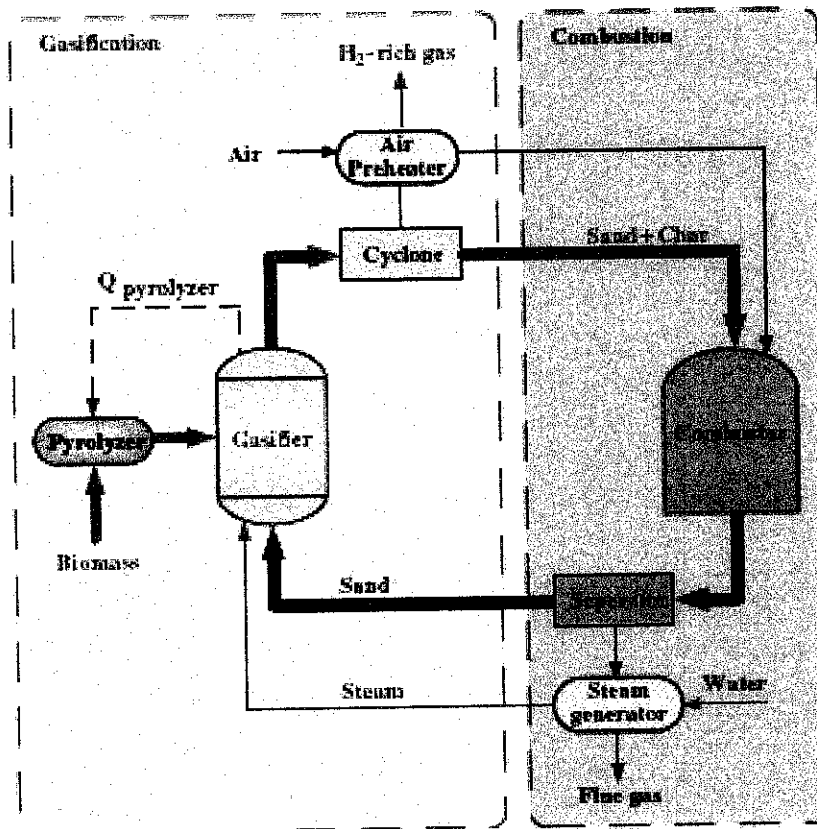


Figure 1: Simulation of biomass gasification in interconnected fluidized beds

Mehrdokht B. Nikoo and Nader Mahinpey had reported in their work entitled, “Simulation of biomass gasification in fluidized bed reactor using ASPEN PLUS” [17] that the hydrogen percentage yield increased from 39-43% for temperature range of 700-900°C. The hydrogen percentage yield decreased from 40-38% for equivalence ratio (ER) value range of 0.19-0.27. The results also showed that the hydrogen percentage yield increased from 38-40% for steam/biomass ratio range of 0-4. The gasification process was simulated using ASPEN PLUS in a fluidized bed reactor system with steam as the gasification medium.

The following assumptions were considered in modeling the gasification process;

- a) Steady state and isothermal process.
- b) Biomass devolatilization takes place instantaneously.
- c) All gases are uniformly distributed within the emulsion phase.
- d) Particles are spherical and of uniform size and the average diameter remain constant during gasification.
- e) Char only contains carbon and ash.
- f) Char gasification starts in the bed and completes in the freeboard.

The experimental setup parameters used in the simulation were;

Table 3: Operating conditions of the gasification process

Reactor temperature	700-900°C
Reactor pressure	1.05bar
Air temperature	65°C
Air flow rate	0.5-0.7 N m ³ /h
Steam temperature	145°C
Steam flow rate	0-1.8 kg/h
E_a/R (combustion)	13523K
k (combustion)	0.046/s.atm
E_a/R (steam gasification)	19544K
k (steam gasification)	6474.7/s.atm

$$ER = \frac{\text{WeightOxygen(Air)}/\text{WeightDryBiomass}}{\text{StoichiometricOxygen(Air)}/\text{BiomassRatio}}$$

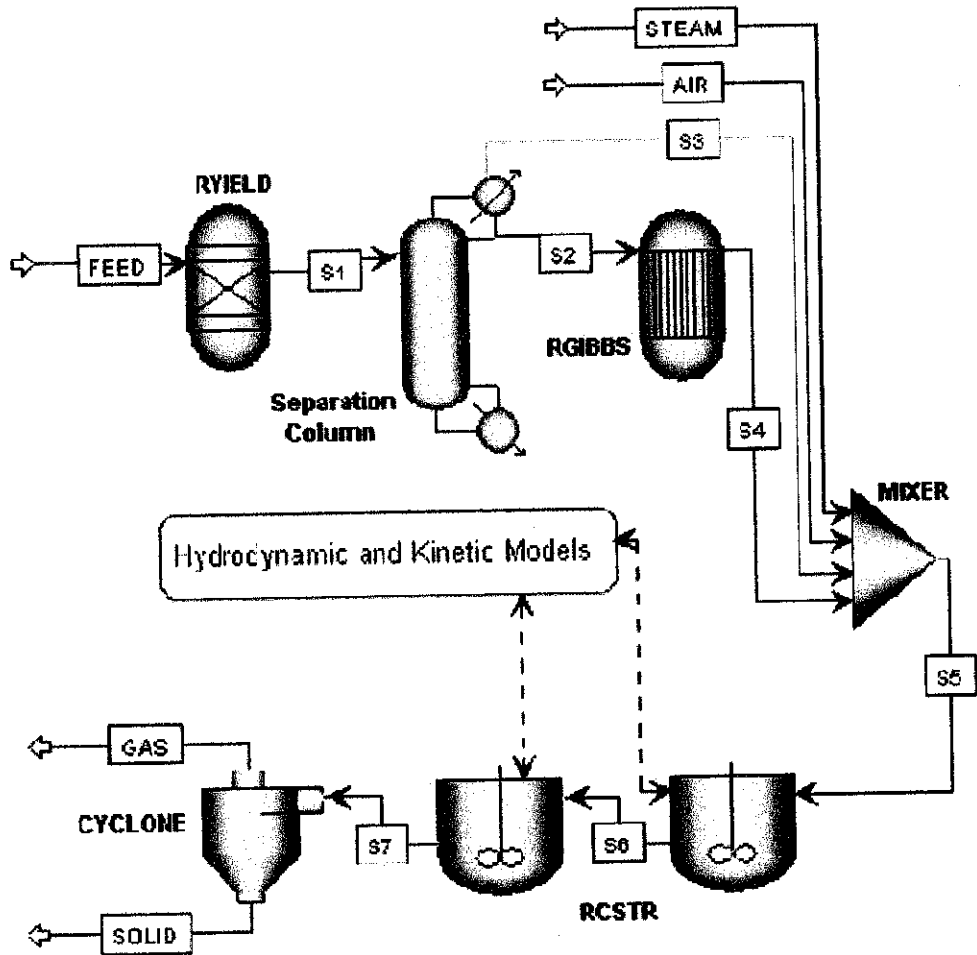


Figure 2: Comprehensive simulation diagram for the fluidized bed gasification system

Tobias Proll and Hermann Hofbauer had reported in their work entitled, **“H₂ rich syngas by selective CO₂ removal from biomass gasification in a dual fluidized bed system – Process modeling approach”** [19] that the results from the simulation for equal fuel power (8000kW) used by both conventional process and selective CO₂ transport plant showed the variation of H₂ amount in product gas with the fuel water content. The maximum production of H₂ for the conventional plant is observed for the fuel that has 50wt% water content with only 45v/v% of H₂ in the product gas. Whereas, the maximum production of H₂ for the selective CO₂ transport plant is observed for the fuel that has 40wt% water content with 84v/v% of H₂ in the product gas. The gasification process was simulated using IPSEpro in a dual fluidized bed reactor system with steam as the gasification medium.

The gasification is investigated for the special case that CaO/CaCO₃ is used as bed material allowing selective transport of CO₂ from the gasification reactor to the combustion reactor by repeated carbonation and calcinations. The selective transport of CO₂ results in high H₂ contents in the produced syngas. The conventional system operates with natural olivine as catalytically active bed material at temperature of about 850-900°C in the gasification reactor.

The assumptions that are made for the simulations were;

- a) The steps of drying and devolatilization are completed first within the gasification reactor releasing the main part of the product gas compounds.
- b) Heterogeneous char gasification reactions determine the degree of char conversion and therefore the degree of total fuel conversion.
- c) The kinetics of the steam gasification reaction, $C + H_2O \leftrightarrow CO + H_2$ can be considered to be the fastest carbon gasification reaction and thus the kinetics of the reaction may be applied to determine the amount of residual char leaving the gasifier with the circulating bed material towards the combustion reactor.

Table 4: Constant process parameters during the simulation runs

Parameter	Unit	Conventional	CO ₂ transport
P_{th}	kW	8000	8000
$Q_{loss,G}$	kW	40	30
$Q_{loss,R}$	kW	160	150
T_G	°C	900	645
T_R	°C	954	900
$m_{Fluid,G}$	kg/h	500	500
λ_R	-	1.12	1.12
$T_{Fluid,G}$	°C	450	450
$T_{A,R}$	°C	450	450
$w_{CaO,bed}$	kgCaO/kg	0.0	0.9
$w_{Oliv,bed}$	kg/kg	1.0	0.1
$k(T_G)$	s ⁻¹	0.175	0.0228
$p\delta_{Eq,COshift}$	-	0.0	-0.5

where	P_{th}	fuel power of the entire gas generation unit based on LHV
	$Q_{loss,G}$	heat loss in the gasification reactor
	$Q_{loss,R}$	heat loss in the combustion reactor
	T_G	temperature in the gasification reactor
	T_R	temperature in the combustion reactor
	$m_{Fluid,G}$	mass flow of the fluid in the gasification reactor
	λ_R	air ratio of combustion in the gasification reactor
	$T_{Fluid,G}$	fluid temperature in the gasification reactor
	$T_{A,R}$	air temperature in the combustion reactor
	$w_{CaO,bed}$	mass fraction of CaO in the bed
	$w_{Oliv,bed}$	mass fraction of olivine in the bed
	$k(T_G)$	kinetic constant of fuel conversion in the gasifier
	$p\delta_{Eq,COshift}$	logarithmic equilibrium distance for CO shift reaction

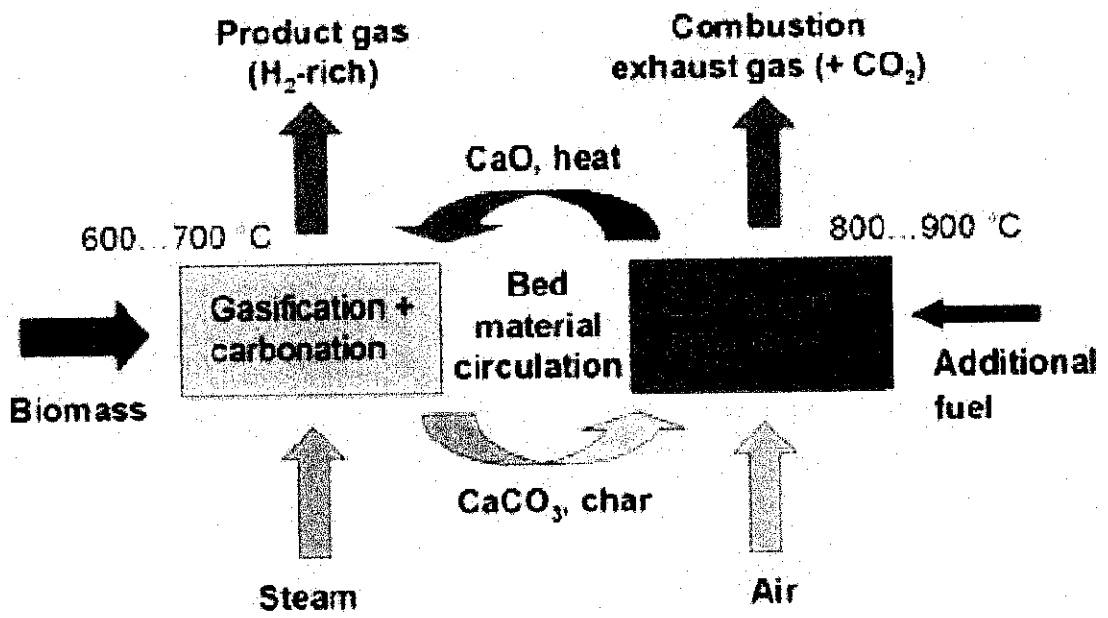


Figure 3: Steam gasification with selective transport of CO₂

P. Spath, A. Aden, T. Eggeman, M. Ringer, B. Wallace and J. Jechura had reported in their report entitled, “**Biomass to Hydrogen Production Detailed Design and Economics Utilizing the Batelle Columbus Laboratory Indirectly-Heated Gasifier**” [20] that a gas yield of 0.04 lb-mole dry gas/lb biomass would be obtained for a temperature of 870°C and a pressure of 1.6 bar with the steam-to-biomass ratio of 0.4 lb biomass/lb biomass. The gasification process was simulated using ASPEN PLUS in a circulating fluidized bed reactor system with steam as the gasification medium.

Table 5: Operating conditions of the gasification process

Gasifier temperature	870°C
Gasifier pressure	1.6bar
Steam/biomass (bone dry) ratio	0.4 lb steam/lb biomass
Sand purge rate	0.1wt% of circulation rate
Gas yield	0.04 lb-mole of dry gas/lb biomass (bone dry)
Char yield	0.22 lb/lb biomass (bone dry)
H ₂ /CO ratio	0.57

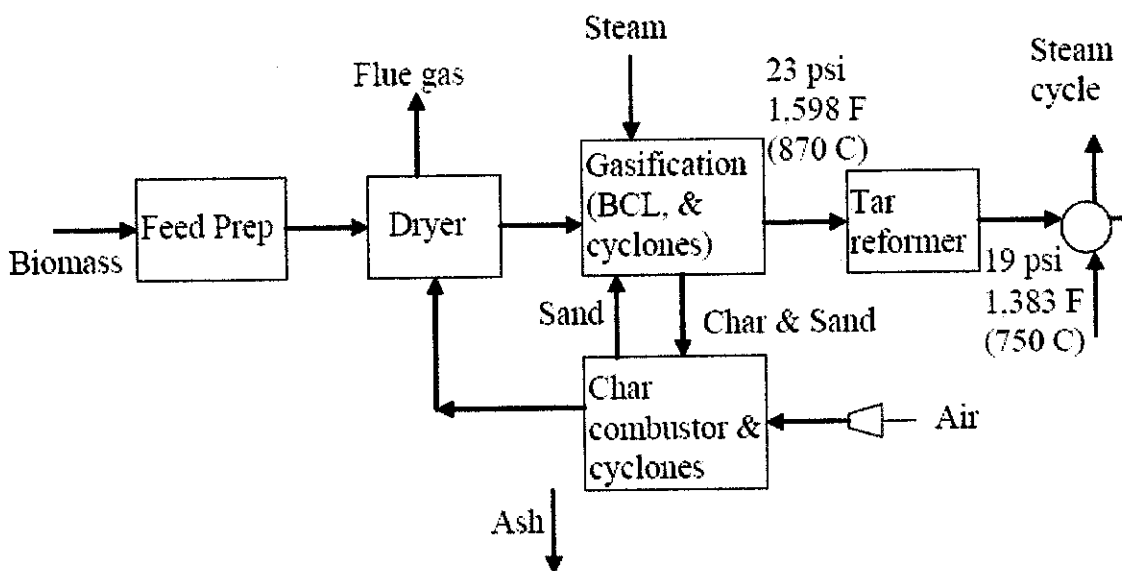


Figure 4: Part of the block diagram of the gasification process

Table 6: Summary of literature review gasification simulation results

Source	Simulation software	Gasifier temperature, T_G ($^{\circ}\text{C}$)	Combustor temperature, T_c ($^{\circ}\text{C}$)	Gasifier pressure (atm)	Gasification medium	H_2 yield
[8]	ASPEN PLUS	650-900	920	0.987	Steam	54-63g H_2 per kg biomass ($T_G=750\text{-}800^{\circ}\text{C}$, steam/biomass ratio=0.6-0.7)
[17]	ASPEN PLUS	700-900	-	1.036	Steam	39-43%
[19]	IPSepro	645	900	-	Steam	84v/v% of H_2 (40wt% water content of fuel)
[20]	ASPEN PLUS	870	-	1.579	Steam	23.85% (Steam/biomass ratio=0.4)

CHAPTER 3

3. METHODOLOGY

3.1 Project Methodology

1) Problem statement / definition

The problems are clarified and broken down to several main parts so that they would be easier to be solved by parts.

2) Literature review / research

Research is done to find process alternatives for the EFB gasification process. Research is focused onto the literatures that implement similar approaches and is extended towards finding new technologies to improve the gasification process. Data such as the gasification temperature, pressure, medium, steam-to-biomass ratio and the expected hydrogen yield that will be obtained for such operating conditions are collected.

3) Alternative selection and comparison

The alternatives that are obtained earlier are gathered together and comparison between those alternatives with the same basis is made. The practicability of the alternatives is taken into consideration as well as the advantages and disadvantages of selecting those alternatives.

4) Solution synthesis

From the selected alternative, a basic process flow which emphasizes on the major parts of the process is established. An actual representation of the process flow is then developed from the basic process flow. Using the developed flowsheets, the work flow is established in iCON.

5) Solution implementation

The simulation is done using iCON at different operating conditions. iCON is a PETRONAS owned Process Simulation Software which is at par with commercial process simulators; e.g. HYSYS, UNISIM, PRO-2, etc.. iCON was launched in 2004 and has been widely used throughout PETRONAS OPU's. The process conditions are determined with the guidance from the information extracted from the literature reviews. Several simulations with different process conditions are done to attain a specific trend of the variations.

6) Results analyses and discussions

The simulation results are analyzed and the optimum process conditions are determined. The analyses are focused on the variation of product gas compositions with steam-to-biomass ratio, the variation of product gas compositions with temperature and the variation of hydrogen yield with temperature.

7) Conclusions

The technical and economical feasibility of the gasification process is concluded. As per economical aspect, the first-level economic potential of the process is determined.

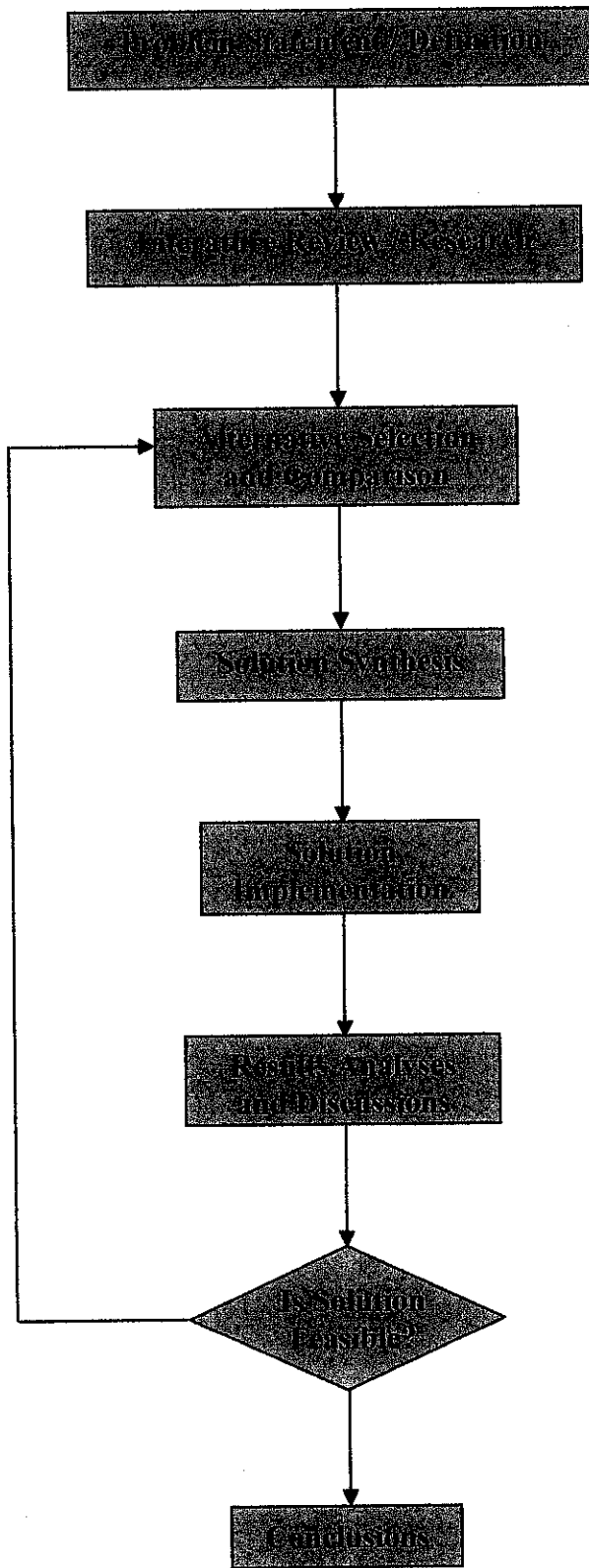


Figure 5: Research methodology

No.	Activities	W1	W2	W3	W4	W5	W6	W7	W8	W9	W10	W11	W12	W13
1	Topic Selection, Problem Statement/ Definition, Gather Literatures													
2	Literature Review / Research													
3	Submission of Preliminary Report													
4	Alternatives Process Routes Selection and Comparison													
5	Solutions Synthesis (Benchmark from Existing Technologies, Establish Basis for The Simulation Process Flow													
6	Submission of Progress Report													
7	Seminar 2 (Internal Examiner)													
8	Solution Implementation (Setup of Simulation in iCON)													
9	Submission of Interim Report Final Draft													
10	Oral Presentation													

Figure 6: Project Gantt chart (Part 1)

No.	Activities	W1	W2	W3	W4	W5	W6	W7	W8	W9	W10	W11	W12	W13	W14	W18	W20
1	Briefing																
2	Solution Implementation (Simulation work using iCON)																
3	Submission of Progress Report 1																
4	Results Analyses and Discussions																
5	Submission of Progress Report 2																
6	Conclusions and Recommendations																
7	Poster Exhibition/Pre-EDX																
8	EDX																
9	Report Modifications																
10	Submission of Final Report (Softcopy and Softbound)																
11	Final Oral Presentation																
12	Submission of Final Report (Hardbound)																

Figure 7: Project Gantt chart (Part 2)

3.2 Process Screening

The first step that is done in accordance to establish the process flow diagram of the gasification process is to identify the gasification methods that would probably provide better results in terms of the quality of the product gas. For this purpose, the comparisons between air gasification and steam gasification are based on a research that has been done by Gonzalez et al. [23].

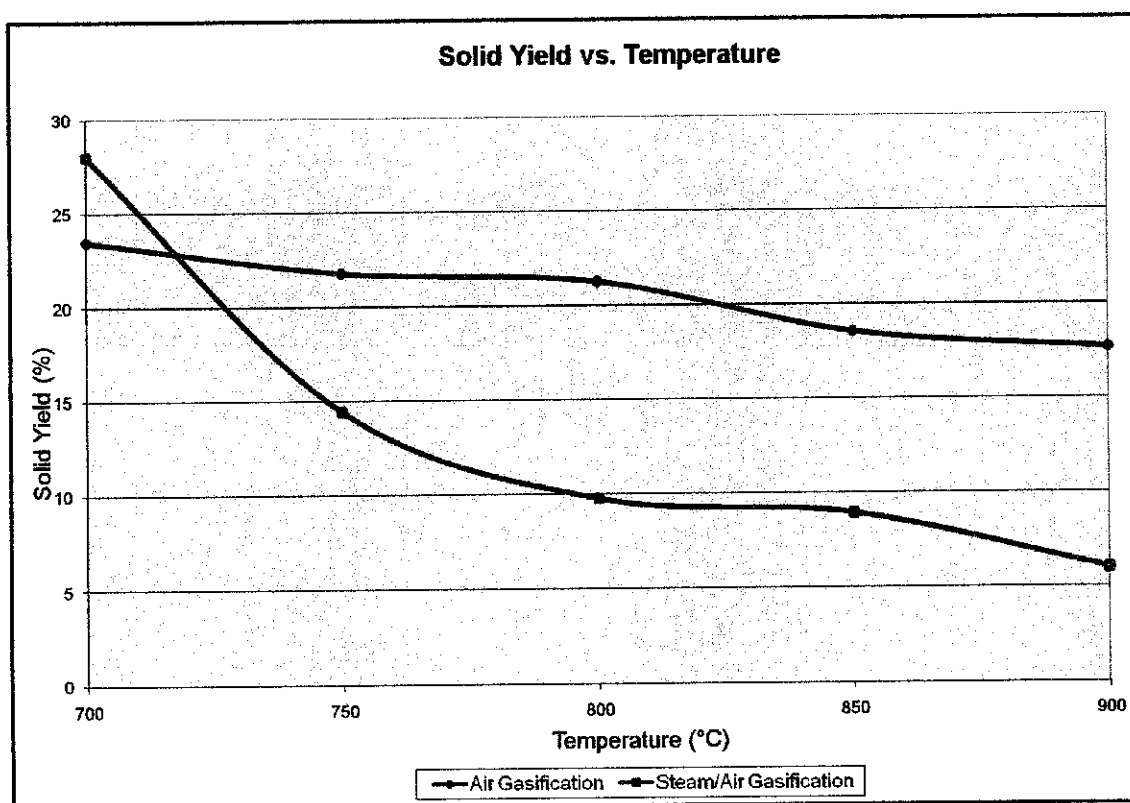


Figure 8: Comparison of solid yields between air and steam gasification [23]

Generally, the solid yield decreases as the gasification temperature increases. For a range of temperature from 700-900°C, the solid that is produced from the air gasification is significantly higher than that of the steam gasification. The impact of temperature variations towards the solid yields from the air gasification are not as significant compared to the steam gasification. The solid yield decreases from 23% to 18% for air gasification whereas for steam gasification, the solid yield decreases from

28% to 6%. This shows that the steam gasification provides better performance in terms of product gas treatment compared to the air gasification.

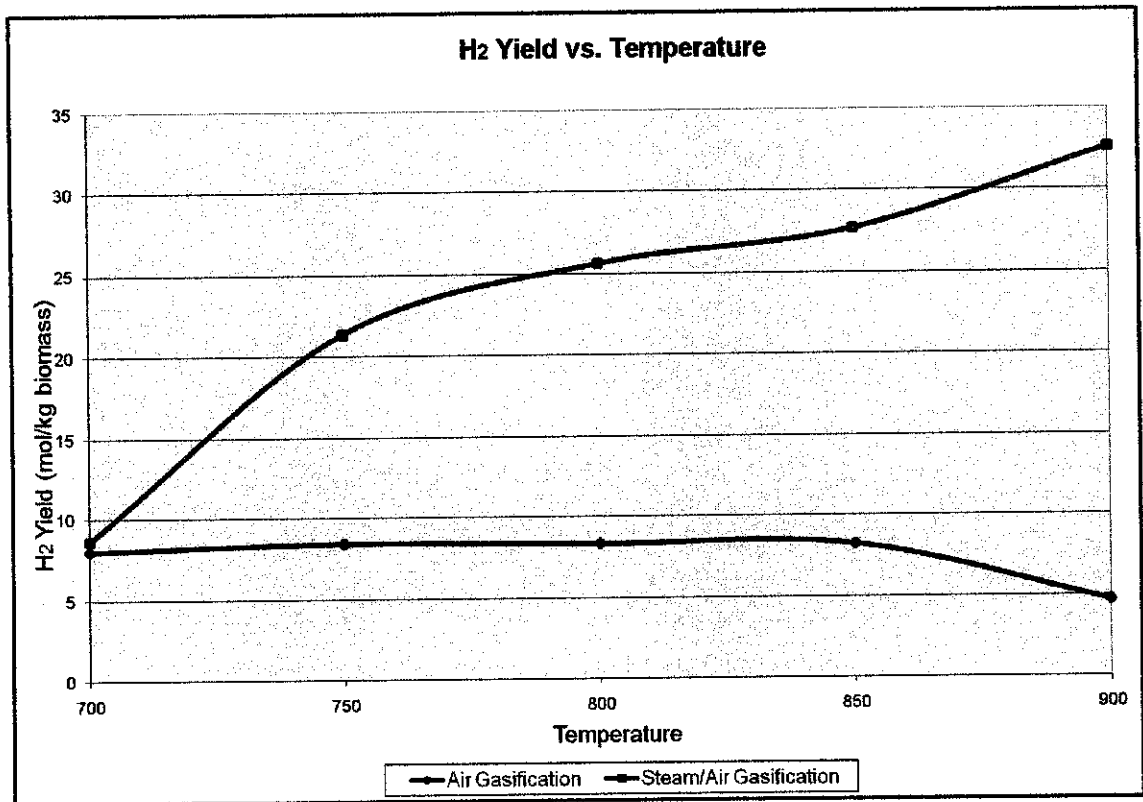


Figure 9: Comparison of H₂ yields between air and steam gasification [23]

Similarly, for the same temperature range the hydrogen yield for steam gasification is also higher compared to the air gasification. The hydrogen yield for air gasification decreases with temperature from 850-900°C. On the other hand, the hydrogen yield for steam gasification increases considerably from 8% to 33% for the same temperature interval. This shows that the steam gasification process would lead to a higher yield of hydrogen compared to the air gasification process.

3.2.1 Comparisons between fixed bed and fluidized bed gasifier

The second step is to determine the type of gasifier that is suitable for the gasification process. There are 2 main types of gasifiers considered which are the fixed bed gasifier and the fluidized bed gasifier. Table 13 shows the significant differences that both systems possess;

Table 7: The comparison between fixed bed gasifier and fluidized bed gasifier [22]

Fixed bed	Fluidized bed
Internal moving parts with some mechanical complications	No moving parts
Bad temperature distribution	Good temperature distribution
Hot spots with exothermic reaction	No hot spots
Poor heat exchange	Very good heat exchange
Channeling is possible	Good gas solid contact and mixing
Residence time: Solids (hours to days), Gas (seconds)	Residence time: Solids (seconds to minutes), Gas (seconds)
Low pressure drop	High pressure drop
High residence time of solids	High reaction rates, low residence time of solids
Very limited scale-up potential	Very good scale-up potential
Long heat-up period	Easy to start and stop
Limitation of fast change of fuels with different calorific values, high fuel content in bed	Fast change of different fuels, low fuel content in the bed. Inventory of solid carbon is lowered by the high content of inert material in the bed
More space required for high throughput	Less space requirement
Stringent size specification required for feedstock	Variety of particle sizes can be handled

Large and uniform sized pellets needed	Wide particle size distribution
Feedstock fine particles have to be handled separately	High fine particles content acceptable
Product gas contains tar, oil, phenols and ammonia (updraft), Low amount of tar and phenols in product gas (downdraft)	Low amount of tar and phenols in product gas
Low ash carry over	Higher particulates in product gas
Low dust content in product gas (updraft), High dust content in product gas (downdraft)	Inevitable loss of carbon in ash due to the non-uniform solids composition of the bed
Extensive product gas cleanup needed (updraft), Relatively clean product gas is produced (downdraft)	High dust content in the gas phase
No primary gas cleaning possible	Primary gas cleaning possible
Molten slag possible	Ash not molten
High investment for high loads	Low investment

Red: Disadvantage

Blue: Advantage

From the above comparison, it is obvious that the better choice of gasifier is the fluidized bed gasifier and in real life, the fluidized bed gasifier is mostly used in the industry for the gasification process.

3.2.2 Selection of type of fluidized bed gasifier

The third step is to compare between the different types of gasifiers that are available in the chosen class of gasifier; in this case the fluidized bed gasifier. Simplified process flow diagrams are established from the conclusion from various literatures.

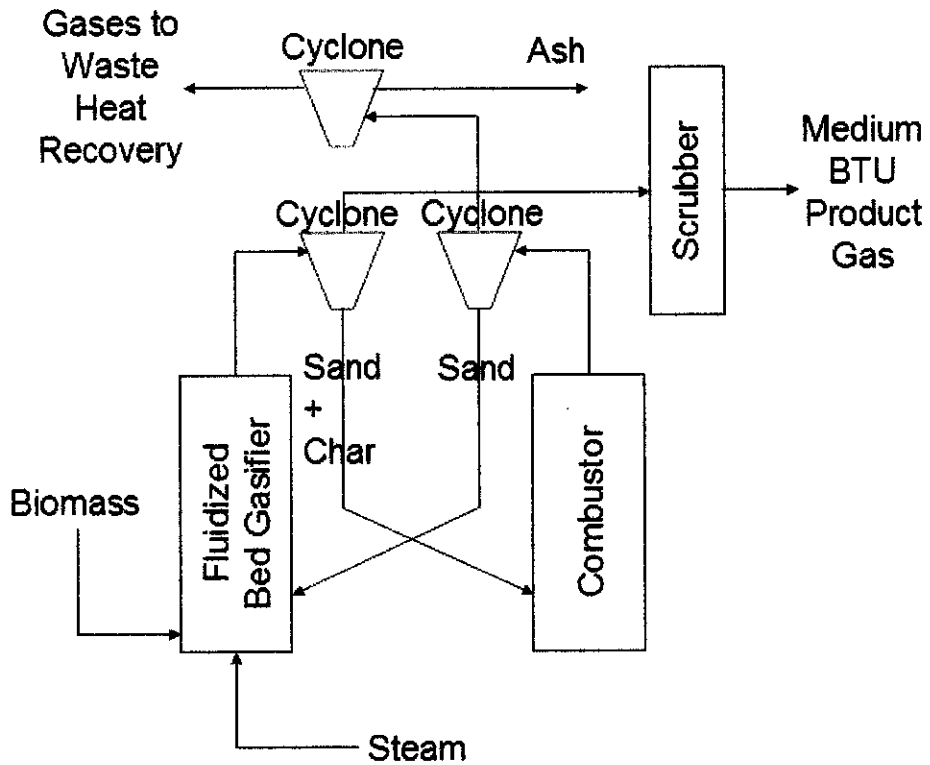


Figure 10: Circulating fluidized bed gasifier system [10]

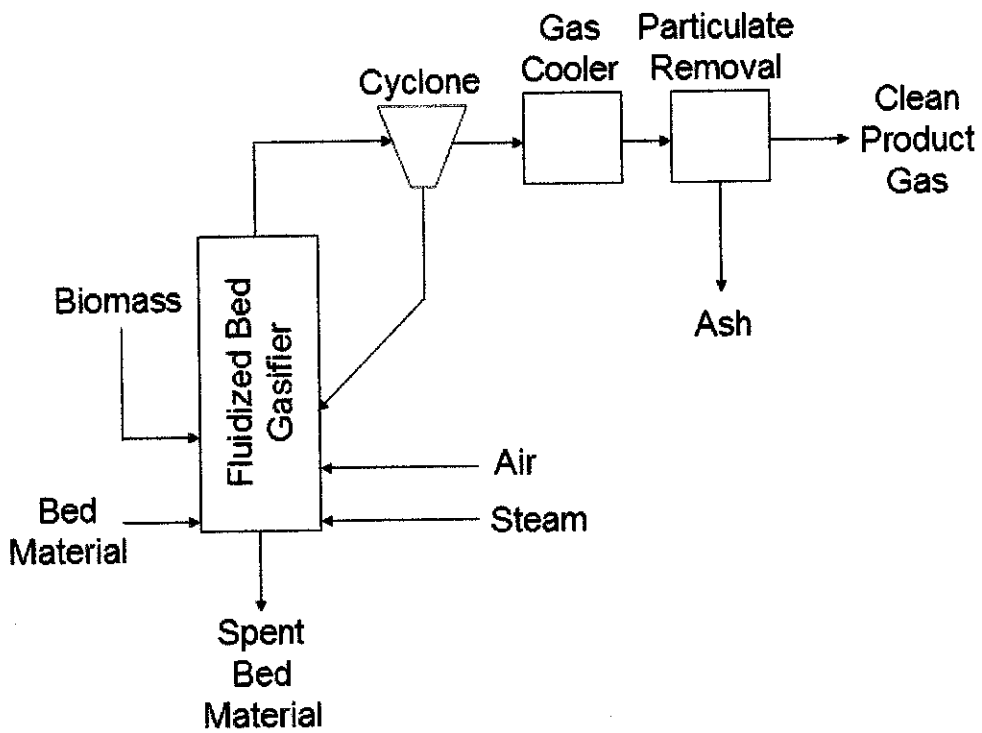


Figure 11: Bubbling fluidized bed gasifier system [10]

Table 8: Comparison between bubbling and circulating fluidized bed [15]

Bubbling Fluidized Bed	Circulating Fluidized Bed
Lower pressure drop	Higher pressure drop
Fast heat up	Very fast heat up
Particulate loading: 2-20 g/N m ³	Particulate loading: 10-35 g/N m ³

From the above comparison, the bubbling fluidized bed reactor is chosen due to the fact that it provides lesser pressure drop compared to the circulating fluidized bed reactor.

3.3 Process Development

The basis of the gasification process considered for this project has essentially 3 main steps which are the EFB steam gasification, the carbon dioxide removal with calcium oxide and lastly the regeneration step of calcium oxide.

The feed entering the process is taken as dried EFB with trace moisture content and would first be fed to the gasifier together with oxygen and steam. The gasifier is a bubbling fluidized bed reactor with calcium oxide as the bed material. Parallel to the reactions that occur in the gasifier, carbon dioxide adsorption via reaction with calcium oxide producing calcium carbonate also occurs simultaneously. Preliminarily, the reaction of carbon dioxide with calcium oxide is assumed to occur in uni-directional and goes to completion.

The calcium carbonate formed in the gasifier would be sent to another reactor to regenerate to calcium oxide whereas the product gases would be sent for further treatments. The regeneration reaction is also assumed to occur in uni-direction and goes to completion. The calcium oxide formed from the regeneration reaction would be recycled back to the gasifier whereas carbon dioxide would be sent for disposal. The basic process flow diagram of the overall process is shown in Figure 10;

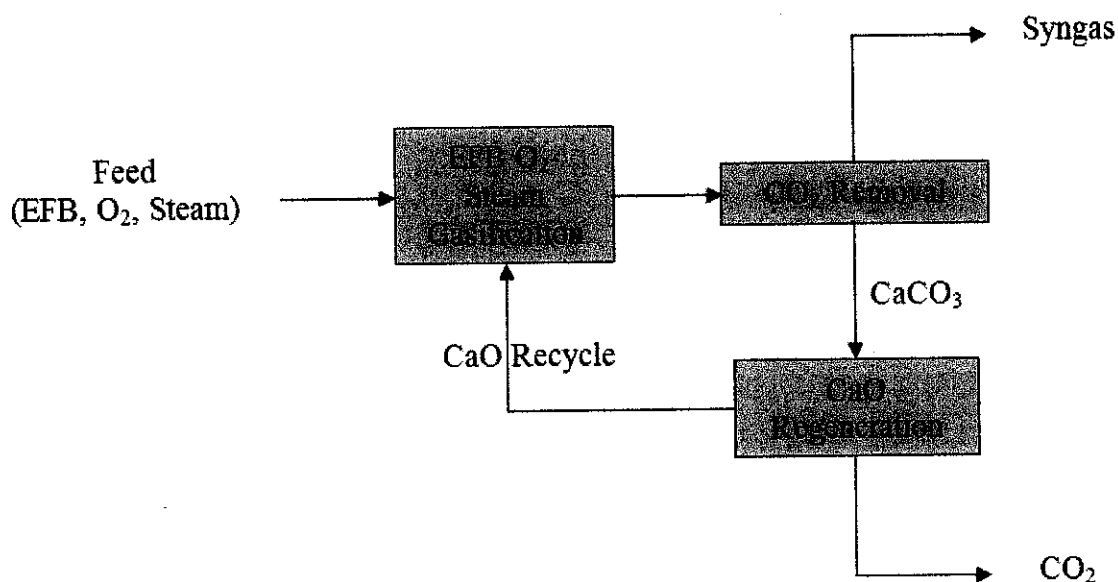


Figure 12: Block diagram for the gasification process flow

From the overall process flow diagram, the basic actual process flow is established as shown in Figure 11;

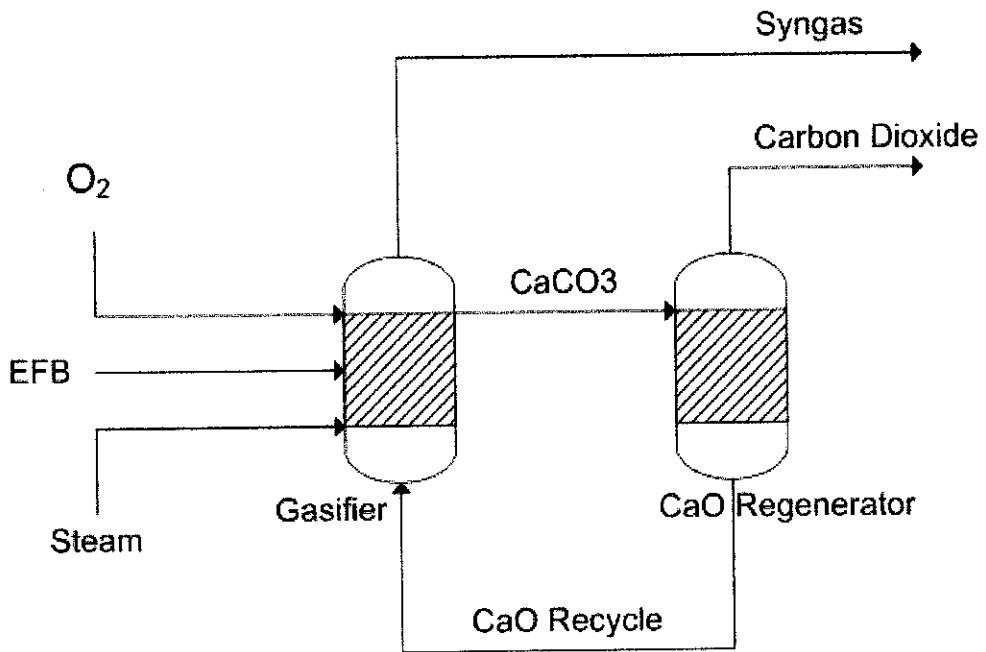


Figure 13: Actual overall process flow diagram of EFB gasification

The overall process flow would be the basis that will be used in order to establish the simulation work flow in iCON.

3.3.1 Process assumptions

Several essential assumptions are made in this project which are;

- The EFB is taken as $C_{3.4}H_{4.1}O_{3.3}$.
- The gasification process occurs in a steady state and reaches the equilibrium.
- The formation of tar is neglected in this process for the simplicity of the simulation.

- d) The combustion is assumed to be uni-directional and goes to completion.
- e) The molar flow rate of EFB and oxygen are fixed at 100 kgmole/hr whereas the molar flow rate of steam depends on the steam-to-biomass ratio.
- f) The integrated gasifier is represented with a gasifier, a water-gas shift reactor, a combustion reactor, a methane reformer, a carbonation reactor, a mixer and a splitter.
- g) The regeneration reactor is represented with a regeneration reactor and a splitter.

3.3.2 Hypothetical development

Several components are not available in the iCON component databases; which are the EFB, calcium oxide and also calcium carbonate. Hence, hypothetical components representing each aforementioned compound are created. The information gathered in order to create the hypothetical components is shown below.

Empty fruit bunch (EFB)

Table 9: Proximate Analysis of the EFB [1]

Elements	wt%
C	49.5
H	5.9
N	0.5
O	40.6
S	0.10
Cl	0.20

Table 10: Properties of EFB

Molecular formula	$C_{3.4}H_{4.1}O_{3.3}$ (based on 1 kg of biomass) [2]
Molecular weight	97.7 kg/kgmole
Bulk density	280 kg/m ³ (at t = 0 week, without any modification or addition) [3]
Moisture content	60% [4]

Calcium oxide**Table 11: Properties of calcium oxide**

Molecular formula	CaO
Molecular weight	56.077 kg/kgmole
Density	3350 kg/m ³
Melting point	2572°C
Boiling point	2850°C
$\Delta H^{\circ}_{f, 298}$	-635.0894 kJ/mol

Table 12: Coefficients for C_p of CaO (T = 298-3200K)

A	49.95403
B	4.887916E-3
C	-3.52056E-7
D	4.6187E-11

$$C_p = A + BT + CT^2 + DT^3 \text{ (J/mol.K)}$$

Calcium carbonate

Table 13: Properties of calcium carbonate

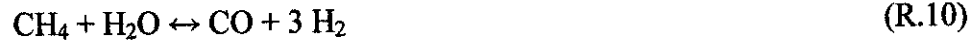
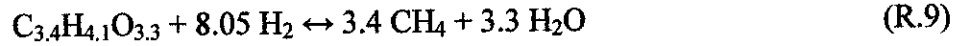
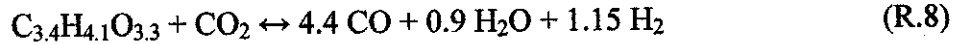
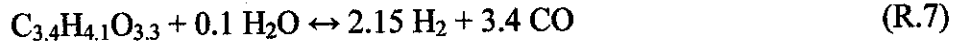
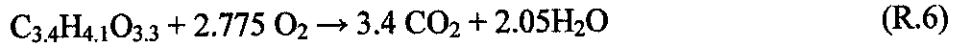
Molecular formula	CaCO ₃
Molecular weight	100.087 kg/kgmole
Density	2710 kg/m ³
Melting point	825°C
Boiling point	~899°C (decomposes)
$\Delta H^{\circ}_{f, 298}$	-1207.6 kJ/mol
C_p	84.0731 J/mol.K

3.3.3 Oxygen-steam gasification reactions

The general reactions that take place for an oxygen-steam gasification reaction reported by Shen et al. [8] are as such;



All of the above reactions are independent reactions, except reaction R.5 (water-gas shift reaction) in which can be considered as the subtraction of R.2 (steam gasification) and R.3 (Boudouard reaction). Based on the previous assumption that EFB is represented with C_{3.4}H_{4.1}O_{3.3}, the balanced gasification reactions specifically for the EFB are written as;



The oxidation reaction is typically assumed to be very fast and goes to completion. Meanwhile, the steam gasification reaction, the Boudouard reaction and the methanation reaction are in equilibrium. The equilibrium constants for some of the above chemical reactions are shown in Table 12. Since there is limited information regarding the reaction kinetics of the gasification reaction of EFB specifically, it is decided that the reaction kinetics for the gasification of coal is used instead. This is based on the research done by Nemtsov et al. [24] which stated that modeling approaches used for coal can serve for biomass gasification as well. The reaction kinetics data is used as of coal and applied to the gasification process of EFB.

Table 14: Kinetic coefficients of gasification reactions

Reactions	$K_{0,i}$	$\Delta\tilde{G}_{0,i} / \tilde{R} \text{ (K)}$	References
R.7	3.139×10^{12}	16344	[6]
R.8	1.238×10^{10}	20294	[7]
R.9	1.435×10^{11}	-11005	[6]

$\Delta\tilde{G}_{0,i}$ = variation of Gibbs function related to reaction i (J/kmol)

\tilde{R} = universal gas constant (8314.2 J/kmol.K)

T_G = gas phase temperature (K)

CHAPTER 4

4. RESULTS AND DISCUSSIONS

4.1 Simulation Process Flow in iCON

The feeds to the gasification process, i.e. EFB, oxygen and steam are flown into a series of reactor systems that are made up as such that it represents, in the actual case as only a single operation which is the gasification reaction in a fluidized bed reactor incorporated with CO₂ adsorption. The whole unit of the gasifier is represented by the gasifier itself, the WGS reactor, the combustion reactor, the methane reforming reactor, the carbonation reactor and also the splitter.

Firstly, the feed would undergo the steam gasification reaction in which the EFB is reacted with steam under certain operating conditions. The aforementioned reaction would produce hydrogen and carbon monoxide and is simulated using an equilibrium reactor. Alongside with the steam gasification reaction process, side reactions such as the Boudouard reaction and the methanation reaction would also take place and are simulated in the same reactor unit.

Secondly, the products from the gasifier are sent to another reactor for the water-gas shift (WGS) reaction to occur. Carbon monoxide would react with water to produce more hydrogen. This reaction is also simulated in an equilibrium reactor.

Next, the products from the WGS reactor are sent to a conversion reactor for the combustion reaction to take place in which the remaining EFB is reacted with oxygen producing carbon dioxide and water.

Then, the product stream from the second reactor would be flowed into another reactor for carbonation reaction to occur. The carbon dioxide in the stream is reacted with calcium oxide producing calcium carbonate and thus resulting in higher hydrogen

content in the final product gases. The hydrogen-rich product gas is first cooled and then treated, cleaned and purified whereas the calcium carbonate is sent to another reactor for regeneration step.

The calcium oxide regeneration reactor is represented by the reactor itself and also a splitter. The regeneration reaction is simulated in a conversion reactor in which the calcium carbonate would desorb the carbon dioxide producing carbon dioxide and calcium oxide. Calcium oxide would then be recycled to the carbonation reactor to be reused as the bed material.

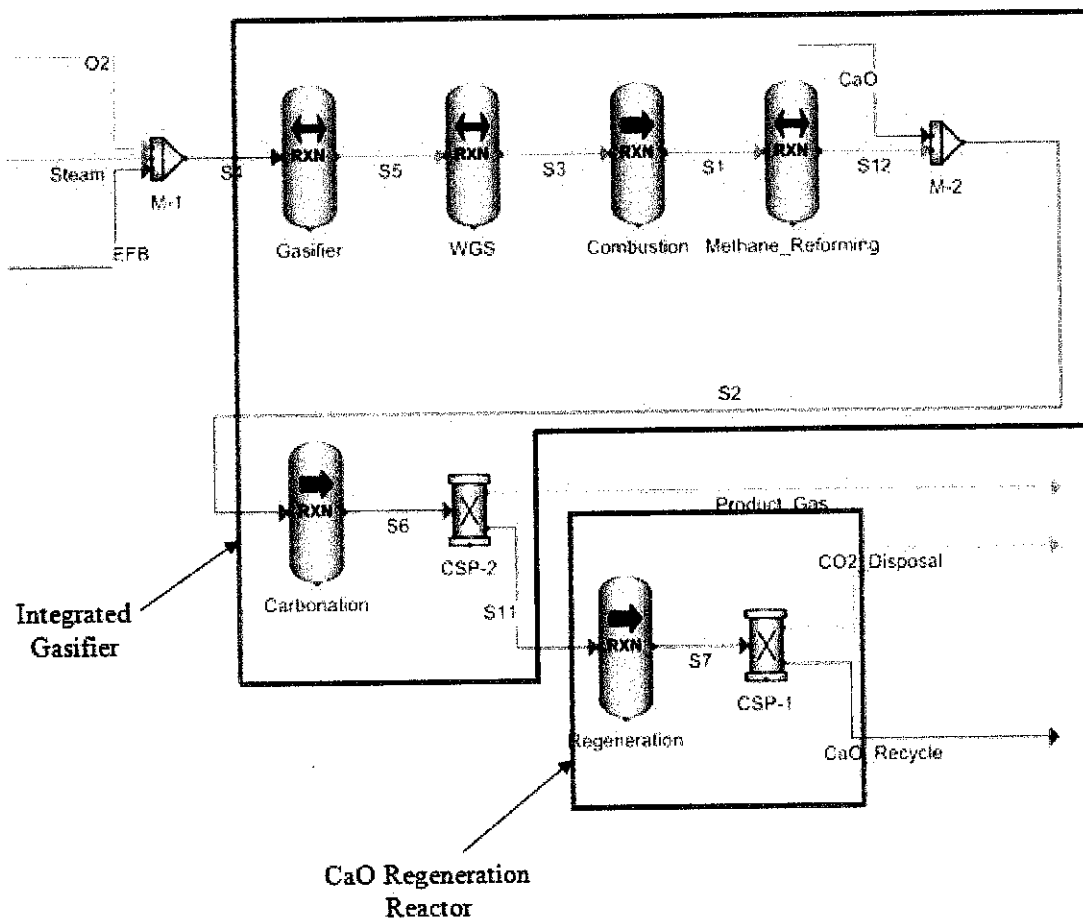


Figure 14: Oxygen – steam gasification process flow

Table 15: Specified reactions for each equipment

Gasifier	$C_{3.4}H_{4.1}O_{3.3} + 0.1 H_2O \leftrightarrow 2.15 H_2 + 3.4CO$
	$C_{3.4}H_{4.1}O_{3.3} + CO_2 \leftrightarrow 4.4CO + 0.9 H_2O + 1.15H_2$
	$C_{3.4}H_{4.1}O_{3.3} + 8.05H_2 \leftrightarrow 3.4CH_4 + 3.3H_2O$
WGS Reactor	$CO + H_2O \leftrightarrow CO_2 + H_2$
Combustor	$C_{3.4}H_{4.1}O_{3.3} + 2.775 O_2 \rightarrow 3.4 CO_2 + 2.05H_2O$
Methane Reformer	$CH_4 + H_2O \leftrightarrow CO + 3H_2$
Carbonation Reactor	$CaO + CO_2 \rightarrow CaCO_3$
Regeneration Reactor	$CaCO_3 \rightarrow CaO + CO_2$

4.2 Syngas Compositions for Different Steam-to-Biomass Ratio

One of the parameters found to significantly affect the syngas compositions is the steam-to-biomass ratio. The ratio is varied from 0.4-0.8 in the simulation and the plots of the syngas compositions versus steam-to-biomass ratio are made.

Table 16: Syngas compositions with steam-to-biomass ratio: 0.4-0.8

Steam-to-EFB ratio	CO (%)	CO₂ (%)	H₂ (%)	CH₄ (%)
0.4	24.320513	0.716353	67.013361	0.161913
0.5	24.598067	0.711479	70.388956	0.347100
0.6	24.631628	0.705360	72.357421	0.546718
0.7	23.487680	0.664870	70.389938	1.846123
0.8	22.337683	0.632660	68.154625	3.087218

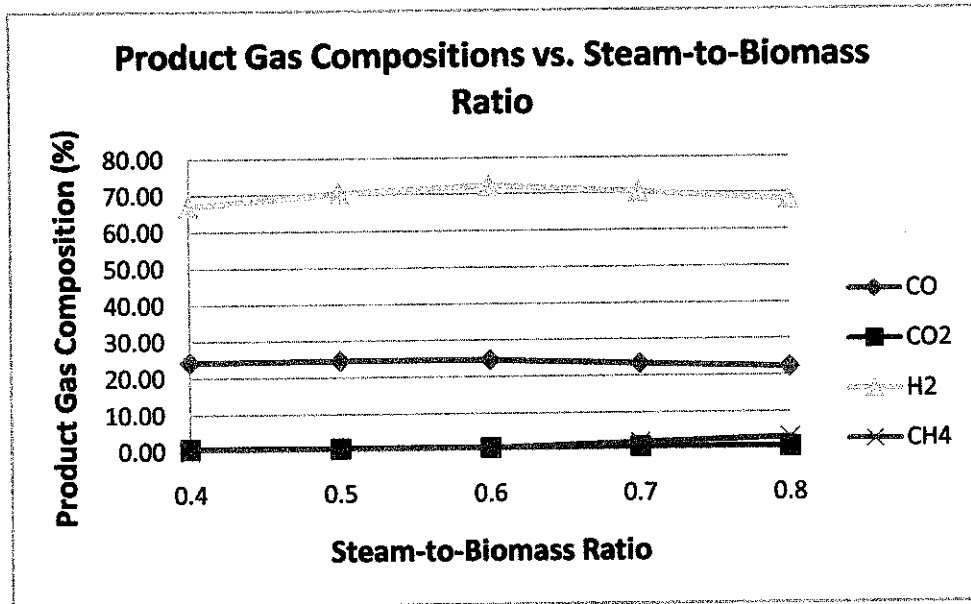


Figure 15: Product gas compositions versus steam-to-biomass ratio plots

From the plots of syngas compositions versus steam-to-biomass ratio above, it can be observed that the highest hydrogen production occurs for the steam-to-biomass ratio around 0.6. This conformed to what has been reported in a literature that the ratio of steam-to-biomass should be between 0.6-0.7 [8].

4.3 Syngas Compositions at Different Gasification Temperature

From the literatures, the most important variable that is found to be manipulating the results of the gasification process is the gasification temperature. The pressure in which the gasification process takes place does not have significant impact on the results obtained. The temperature is varied in the simulation from 600 – 1000°C and the plots of the synthesis gas compositions versus temperature are made. The steam-to-biomass ratio of 0.6 is used for these simulations.

Table 17: Compositions of syngas at T: 600-1000°C

T (°C)	CO (%)	CO ₂ (%)	H ₂ (%)	CH ₄ (%)
600	12.874908	0.947048	39.540174	24.937395
650	16.277345	0.875304	49.499856	17.776407
700	19.067560	0.815597	57.586707	11.956757
750	21.127853	0.772151	63.456088	7.684741
800	22.563728	0.743184	67.420765	4.726203
850	23.556769	0.724561	70.019947	2.703196
900	24.243201	0.713071	71.658040	1.334874
950	24.631632	0.705360	72.357425	0.546721
1000	24.768635	0.697922	72.255768	0.206945

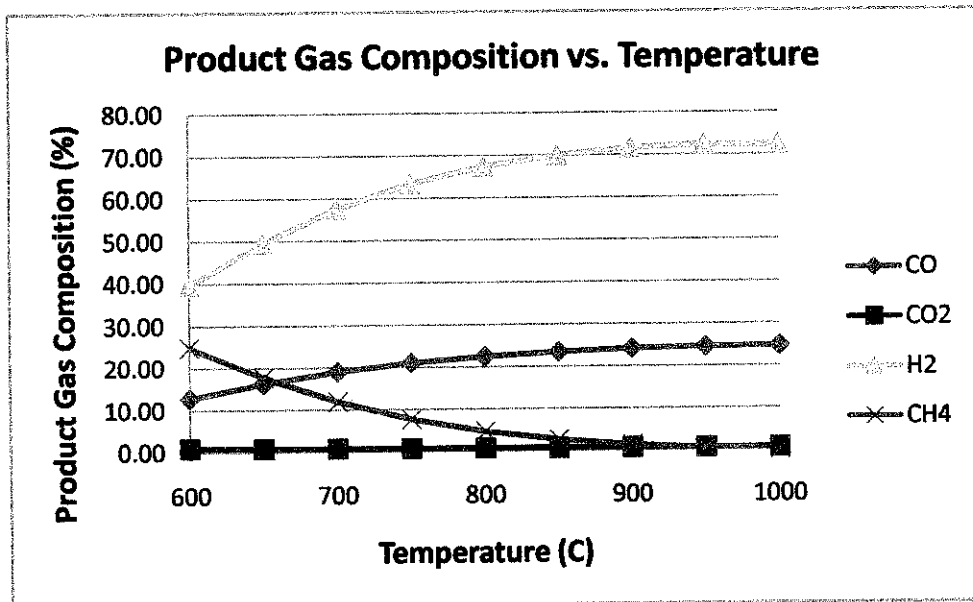


Figure 16: Product gas composition versus temperature plots

From the results above, it is found that the trends of the plots are similar to the work published by Khadse et al. [5]. They have employed the equilibrium model to predict the product compositions of the gasification process for several biomasses such as saw dust, bagasse, subabul and also rice husk. The similarity in the results are found

to be because of that the reactions that are considered in their modelling work were the same as the ones that are considered in this project itself. Above all, this project also employed the reaction equilibrium constants in simulating the gasification process.

Though the trends might be similar, but the values do differ quite dramatically. This is due to the fact that the reaction equilibrium constants are obtained for coal and not particularly EFB. The steam/oxygen ratio is also another contributing factor to the difference in the results obtained for both sides. Moreover, this project is integrated with carbon dioxide adsorption using calcium oxide. Therefore, the final compositions of the syngas, especially for carbon dioxide in this project are different in terms of values compared to the literature.

Despite the dissimilarities between the results obtained compared to the findings by Khadse et al. [5], the results somehow do map out to the findings by Shen et al. [8]. The trends of the syngas compositions do follow the trend in the aforementioned literature. The compositions of the syngas obtained for the same gasification temperature interval are also similar to what is stated in the literature; except for the compositions of carbon dioxide which differs significantly from the literature because of the absence of the adsorption step using calcium oxide. The comparison of the syngas compositions between this project and the work done by Shen et al. [8] is shown in Table 17;

Table 18: Comparison of syngas compositions with literature

	This project	Shen et al.
CO (%)	10 – 25	0 – 20
CO ₂ (%)	0.7 – 1.0	20 – 40
H ₂ (%)	40 – 70	40 – 60
CH ₄ (%)	1 – 25	0 – 20

4.4 Hydrogen Yield at Different Gasification Temperature

Another way to investigate the effect of gasifier temperature on the process of EFB gasification is to observe the hydrogen yield variation with temperature.

Table 19: Hydrogen yield at temperature: 600-1000°C

T(°C)	H ₂ (kg/h)	H ₂ (g/h)	H ₂ yield(g H ₂ /kg EFB)
600	202.6493411	202649.3411	20.74200011
650	276.3899829	276389.9829	28.28966048
700	347.1176484	347117.6484	35.52893024
750	406.0117973	406011.7973	41.55699051
800	450.0064261	450006.4261	46.06002314
850	480.9196547	480919.6547	49.22412024
900	501.3541121	501354.1121	51.31567166
950	511.2325209	511232.5209	52.32676775
1000	512.5017728	512501.7728	52.45668094

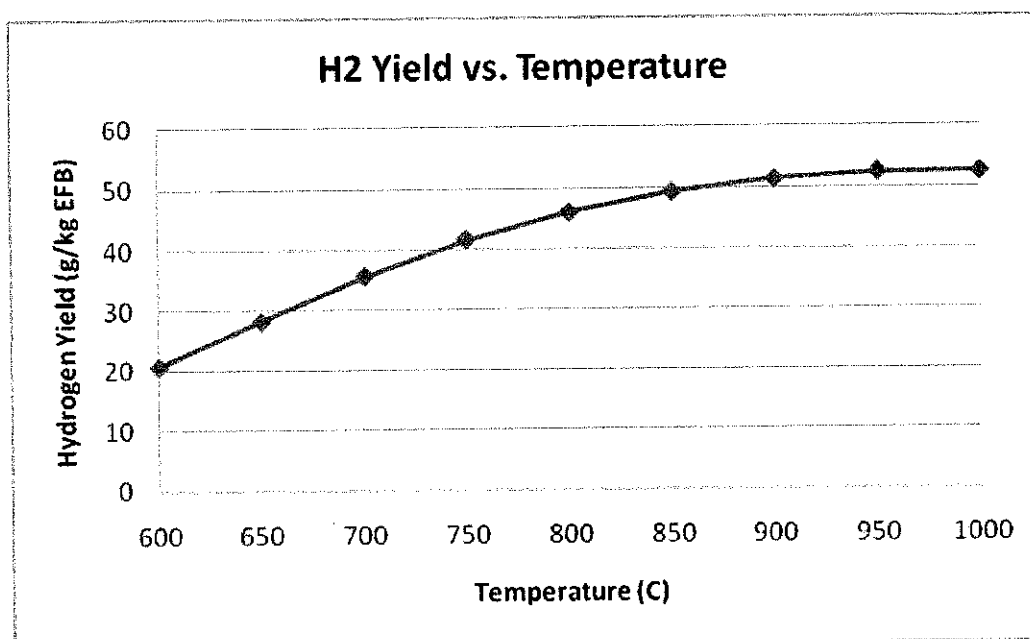


Figure 17: Hydrogen yield versus temperature plots

From the plot of hydrogen yield versus temperature, it is observed that the hydrogen yield is the highest around 950°C and becomes nearly constant beyond that temperature. The comparison of the hydrogen yield with the work done by Shen et al. [8] is shown in Table 20.

Table 20: Comparison of hydrogen yield with literature

	This project	Shen et al.
Temperature (°C)	950	600 – 920
Yield (g H ₂ /kg biomass)	52	54 – 63

4.5 Economic Potential

The feasibility of the project is determined using the economic potential of the first level calculation. The raw material to the process is taken as steam considering that EFB and air is free, and the product for the process is taken as hydrogen. The current prices of steam and hydrogen are as given in Table 18 [12];

Table 21: Products and raw materials data

	Products		Raw Materials	
	Price	Flow rate	Price	Flow rate
Steam	-	-	RM 15.46/MT	1441.22 kg/hr
Oxygen	-	-	RM 92.40/MT	3199.88 kg/hr
Hydrogen	RM 9.71/gallon	26.416 m ³ /hr	-	-

The EP1 calculation is as such;

EP1 = Total Revenue (Products) – Total Cost (Raw materials)

$$\begin{aligned} &= \left[\frac{RM9.71}{gallon} \times \frac{26.416m^3}{hr} \times \frac{1gallon}{0.003785m^3} \right] \\ &\quad - \left[\left(\frac{RM15.46}{MT} \times \frac{1441.22kg}{hr} \times \frac{1MT}{1000kg} \right) + \left(\frac{RM92.40}{MT} \times \frac{3199.88kg}{hr} \times \frac{1MT}{1000kg} \right) \right] \\ &= 67,767.33 - 317.95 \\ &= \mathbf{RM\ 67449.38/hr} \end{aligned}$$

CHAPTER 5

5. CONCLUSIONS AND RECOMMENDATIONS

As a conclusion, the gasification process of EFB can be simulated quite well using iCON and that the results obtained do map out to certain literatures. The integration of the gasification process with adsorption using calcium oxide shows good results in which it yields higher hydrogen content in the product gas. The optimum temperature for the gasification of EFB is 950°C with the optimum steam-to-biomass ratio of 0.6. From the economical point of view, the gasification process is proven to be feasible and has the potential for commercialization.

The recommendation that can be made for this project is that the simulation process flow of the gasification process should be improved and modified. Further work has to be done to find a way to simulate the reactions in a single reactor rather than by parts as done in this project. Currently in this project, the gasification reactions are assumed to reach equilibrium and occur at steady state. Detailed kinetics study on the gasification reaction of specifically EFB has to be done in order to obtain more accurate results. Detailed kinetics study has to be done regarding the adsorption of carbon dioxide using calcium oxide. The kinetics study is important for the purpose of reactor sizing and specification. As an addition, extensive research has to be done regarding the properties of EFB in order to create a more accurate hypothetical component in iCON.

REFERENCES

- [1] Journal of Oil Palm Research Vol. 18, June 2006, p.210-218.
- [2] 2002 International Oil Palm Conference, Nusa Dua, Bali, Indonesia, July 8-12, 2002.
- [3] "The Production of Synthetic Diesel from Biomass", KMITL Sci. Tech. J. Vol. 6, No. 1, Jan.-Jun., 2006.
- [4] "Bio-oil derived from empty fruit bunches", Fuel 87 (2008), p.2606-2613.
- [5] Anil Khadse, Prasad Parulekar, Preeti Aghalayam & Anuradda Ganesh, "Equilibrium Model for Biomass Gasification", Advances in Energy Research 2006.
- [6] Hottel, H.C., Howard, J.B. (1971). New Energy Technology. Cambridge, Massachusetts: MIT Press.
- [7] Parent, J.D., Katz, S. (1948). Equilibrium Compositions and Enthalpy Changes for the Reaction of Carbon, Oxygen, and Steam. IGT-Inst. Gas Tech., Research Bulletin 2.
- [8] Laihong Shen, Yang Gao & Jun Xiao, "Simulation of hydrogen production from biomass gasification in interconnected fluidized beds", Biomass and Bioenergy 32, 2008, p.120-127.
- [9] Stefan Czernik, Robert Evans & Richard French, "Hydrogen from biomass-production by steam reforming of biomass pyrolysis oil", Catalysis Today 129, 2007, p.265-268.
- [10] Peter McKendry, Energy production from biomass (part 3): gasification technologies, Bioresource Technology 83, 2002, 55-63.
- [11] Yong et al., Potential of hydrogen from oil palm biomass as a source of renewable energy worldwide, Energy Policy, 35, (2007).
- [12] Sharina bt. Kamarul Hatta, Personal Communication, Optimal Chemicals (M) Sdn. Bhd., October 2008.
- [13] <http://www.tkk.fi/Units/AES/projects/renew/fuelcell/posters/hydrogen.html>
- [14] Producing Renewable Hydrogen from Biomass, BioCycle, 2004.

- [15] John Rezaiyan & Nicholas P. Cheremisinoff, *Gasification Technologies: A Primer for Engineers and Scientists*, 2005, Taylor & Francis Group.
- [16] Stefan Czernik, Richard French, Calvin Feik, & Esteban Chornet, *Hydrogen from Biomass via Fast Pyrolysis/Catalytic Steam Reforming Process*, 1999.
- [17] Mehrdokht B. Nikoo & Nader Mahinpey, *Simulation of biomass gasification in fluidized bed reactor using ASPEN PLUS*, *Biomass and Bioenergy*, 2008.
- [18] S. Sumathi, S.P. Chai & A.R. Mohamed, "Utilization of oil palm as a source of renewable energy in Malaysia", *Renewable and Sustainable Energy Reviews* 12, 2008, p.2404-2421.
- [19] Tobias Proll & Hermann Hofbauer, *H₂ rich syngas by selective CO₂ removal from biomass gasification in a dual fluidized bed system – Process modeling approach*, *Fuel Processing Technology*, 2008.
- [20] P. Spath, A. Aden, T. Eggeman, M. Ringer, B. Wallace & J. Jechura, *Biomass to Hydrogen Production Detailed Design and Economics Utilizing the Battelle Columbus Laboratory Indirectly-Heated Gasifier*, Technical Report NREL/TP-510-37408, May 2005.
- [21] Suresh Babu, *Biomass Gasification for Hydrogen Production – Process Description and Research Needs*, IEA Bioenergy, 2005.
- [22] Ragnar Warnecke, *Gasification of biomass: comparison of fixed bed and fluidized bed gasifier*, *Biomass and Bioenergy* 18, 2000, 489-497.
- [23] J.F Gonzalez, S. Roman, D. Bragado & M. Calderon, *Investigation on the reactions influencing biomass air and air/steam gasification for hydrogen production*, *Fuel Processing Technology* 89, 2008, 764-772.
- [24] D.A. Nemtsov & A. Zabaniotou, "Mathematical modeling and simulation approaches of agricultural residues air gasification in a bubbling fluidized bed reactor", *Chemical Engineering Journal*, 2008.

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Name: Gasifier Description:

Type: Equilibrium Reactor Gibbs Reactor

Summary | Reactions | Reaction Constants | Settings

Main Data

Name	Value
Energy Out	-272618899.5359
Qdot [W]	
Signal	
Data P [kPa]	0.00

Material

PortName	In	Out
Is Recycle Port	<input type="checkbox"/>	<input type="checkbox"/>
Connected Stream/Unit Op	/54/Dist	/55/In
WgtFrac	0.5629	1.00
T [C]	149.914	1000.00
P [kPa]	300.0	300.0
WgtFlow [kgmole/h]	260.00	375.22
MassFlow [kg/h]	14050.80	14054.95
VolumeFlow [m ³ /h]	1814.007	13230.212
StdVolumeFlow [m ³ /h]	30.003	28.228
StdGasVolumeFlow [SCMD]	1.4762E+5	2.1391E+5

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Inlet gasifier flow specifications

ICONE Steam Gasification, latest - [Gasifier (EquiReactor)]

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Name: Gasifier Description

Type: Equilibrium Reactor Gibbs Reactor

Summary Reactions Reaction Constants Settings

Reactor Name	Rxn0 Steam_Gasification EPR*	Rxn1 Rebound EPR*	Rxn2 Methanation EPR*
CARBON MONOXIDE	3.4	4.4	
WATER	-0.1	0.9	3.3
CARBON DIOXIDE		-1	
HYDROGEN	2.15	1.15	-8.05
METHANE			3.4
CalciumCarbonate*			
OXYGEN		-1	-1
Balance	0.0670	0.0670	0.0670
H.Rxn(25 C)(kJ/mol)	-1.05E+05	-1.27E+05	-8.59E+05

Reaction: 3.0*WATER+3.0*METHANE-3.05*HYDROGEN-1.0*EPR*

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Gasifier reaction specifications

[Icon]: Steam Gasification_test - [Gasifier (LupinReactor)]
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 23 Rabbit Anal 1430 ST
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Name: Gasifier Description: Schematic
 Type: Equilibrium Reactor Gibbs Reactor
 Summary | Reactions | Reaction Constants | Settings
 Equilibrium Constant: K-T Table Phases: Overall
 Calculation Basis: Activities
 Equilibrium Constant - Temperature

Raz0				Raz1				Raz2			
Reaction Constant is 2.6592E-06				Reaction Constant is 1.1949E-07				Reaction Constant is 5.5754E+03			
T (C)	K_eq	K_cal	Error (%)	T (C)	K_eq	K_cal	Error (%)	T (C)	K_eq	K_cal	Error (%)
600.00	7.42E-09	7.42E-09	-0.0014	600.00	6.05E-11	6.05E-11	-1.74E-04	600.00	2.38E+05	2.38E+05	-1.03E-04
700.00	5.09E-08	5.09E-08	0.0062	700.00	8.79E-10	8.79E-10	7.64E-05	700.00	8.15E+04	8.15E+04	-2.21E-04
800.00	2.43E-07	2.43E-07	-0.0110	800.00	6.13E-09	6.13E-09	-1.93E-04	800.00	2.94E+04	2.94E+04	-1.21E-04
900.00	9.90E-07	9.90E-07	0.0063	900.00	3.07E-08	3.07E-08	-1.91E-04	900.00	1.18E+04	1.18E+04	-5.89E-05
1000.00	2.66E-06	2.66E-06	-0.0024	1000.00	1.19E-07	1.19E-07	-3.53E-05	1000.00	5.67E+03	5.67E+03	-1.81E-04

Regression Equation: $K_{cal} = Exp(A + B/T + C \cdot Log(T) + DT)$
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Gasifier reaction kinetics specifications

ICOM - Steam Gasification... [WGS (EqnReactor)]

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Ready

Name: WGS Description: Solved

Types: Equilibrium Reactor Equis Reactor

Summary | Reactions | Reaction Constants | Settings

Main Data

Name	Value	
Energy Out	177.6166	
OutQ [W]	177.6166	
Signal	0.00	
Delta P [Tos]	0.00	

Material

PortName	In	Out
Connected Stream/Unit Op	1.00	1.00
Ve/frac	1000.00	753.1n
T [C]	300.0	300.0
P [Pa]	375.22	375.22
MoleFlow [gmole/h]	14054.95	14054.95
MassFlow [kg/h]	13230.212	13230.212
VolumeFlow [m3/h]	28.228	28.228
StdVolumeFlow [SCMH]	2.1336E+5	2.1336E+5

* Properties (Alt+R)
 * Fraction [fraction]
 * MassFraction [fraction]
 * StdVolumeFlow [fraction]
 * MoleFlow [gmole/h]
 * MassFlow [kg/h]
 * StdVolumeFlow [m3/h]

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WGS reactor inlet specifications

5: COH: Steam Gasification... [WGS (EmpReaction)]

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Ready Name: WGS Description:

Type: Equilibrium Reactor Gibbs Reactor

Summary Reactions Reaction Constants Settings

Item Name	Stoichiometric Coefficient
WATER	-1
CARBON MONOXIDE	1
CARBON DIOXIDE	1
HYDROGEN	1
METHANE	1
CalciumOxide*	
CalciumCarbonate*	
EP3*	
OXYGEN	0.00
Balance	
H Reacts: C[O] (mol)	-41025.49

WGS: 1.0*CARBON_DIOXIDE+1.0*HYDROGEN+1.0*CARBON_MONOXIDE+1.0*WATER

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WGS reactor reaction specifications

(COM) Steam Gasification_latest - [WGS (EquiReactor)]
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Name: WGS Description: Schematic

Type: Equilibrium Reactor Gibbs Reactor
 Summary | Reactions | Reaction Constants | Settings

Equilibrium Constants: K-T Table
 Calculation Basis: Vapor Partial Pressure Units: [K]

Equilibrium Constant - Temperature

Rxn0				
Reaction Constant: 6.223947E+01				
T (C)	K_exp	K_cal	Error (%)	
600.00	93.04	93.04	-2.04E-05	
700.00	58.39	58.39	-7.59E-05	
800.00	39.97	39.97	2.78E-05	
900.00	28.19	28.19	-6.87E-05	
1000.00	22.95	22.95	-2.00E-05	

Regression Equation: $K_{cal} = Exp(A + B/T + C \log(T) + DT)$

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WGS reactor reactions kinetics specifications

6: (COM) Steam Gasification_latest - [Combustion] (Combustion) [ComReactor]

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Ready

Names: Combustion Description: Schematic

Type: Use Reaction Order Simultaneous Reaction

Summary: Reactions Parameters

Main Data

Name	Value
Energy Out	31251143.9759
OutQ [W]	
Delta P [Pa]	0.00
Revd_Conversion [Fraction]	0.9700

Material

Port Name	In	Out
In Recycle Port		
Connected Stream/Link Op	753.Out	Connected to...
Vel [m/s]	1.0	Sheet 1 / Stream S3
T [C]	1000.0	Port : Out
P [Pa]	900	
MassFlow [kg/s]	375.2	
VolumeFlow [m3/s]	1408.95	14657.36
StdVolumeFlow [m3/s]	13230.212	15276.595
StdVolumeFlow [m3/s]	26.228	21.134
StdVolumeFlow [SCMD]	2.1334E+5	2.4766E+5

* Properties (all+r)
 * Fraction [Fraction]
 * MassFlow [kg/s]
 * StdVolumeFlow [m3/s]
 * StdVolumeFlow [SCMD]

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Combustion reactor inlet specifications

ICOM: Steam Gasification... [Methane Reforming (EquiReactor)]
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Name: Methane Refor **Description:** Schematic

Types: Equilibrium Reactor Gibbs Reactor

Summary **Reactions** **Reaction Constants** **Settings**

Main Data

Name	Value
Energy Out	-5019406.6997
Q/KQ [W]	
Signal	
Data P [kPa]	0.00

Material

PortName	In	Out
Is Recycle Port	<input type="checkbox"/>	<input type="checkbox"/>
Connected Stream/Unit Op	/51_Out	/512_In
VarFrac	1.00	1.00
T [C]	1000.00	1000.00
P [kPa]	300.0	300.0
MolarFlow [kmol/h]	435.58	594.36
MassFlow [kg/h]	14057.36	14057.36
VolumeFlow [m ³ /h]	15376.595	21051.702
SolidVolumeFlow [m ³ /h]	21.134	37.698
SolGasVolumeFlow [SCMG]	2.4766E+5	3.3827E+5

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Methane reformer inlet flow specifications

ICON: Steam Gasification Latest - [Methane Reforming (RxnReactor)]

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Ready

Name: Methane Refor Description: Schematic

Type: Equilibrium Reactor Gibbs Reactor

Summary Reactions Reaction Constants Settings

Run Name	Reform
Base Comp	METHANE
CARBON MONOXIDE	-1
WATER	
CARBON DIOXIDE	3
HYDROGEN	-1
METHANE	
CalciumOxide*	
CalciumCarbonate*	
FFI*	
OXYGEN	
Balance	0.00
[H2O]25 = [C]11meol]	2.08E+05

Reforming: 1.0*CARBON MONOXIDE+3.0*HYDROGEN-1.0*WATER-1.0*METHANE

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Methane reformer reaction specifications

(Icon: Steam Gasification_latest - [Methane Reforming (EquilReactor)]
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 20 Rabbit Road 1430 SI
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Name: Methane Refor Description
 Type: Equilibrium Reactor Gibbs Reactor
 Summary | Reactions: Reaction Constants Settings
 Equilibrium Constant:
 Calculation Basis:
 Equilibrium Constant - Temperature
 Reaction Name: Equilibrium Constant
 Bond: 9121.12

Equilibrium Constant: $K = \text{Exp}(\text{Reaction Free Energy})/RT$
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Methane reformer reaction kinetics specifications

iCON: Steam Gasification_latest - [Carbonation (CompReaction)]
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 23 Rabbit Award 1430 SI
 Finished recalling case (C:\Documents and Settings\Guest\My Documents\ERB Gasification\Steam Gasification_1oktest.vmp, Uncompressed w

Name: Carbonation Description: Schematic
 Type: Use Reaction Order Simultaneous Reaction

Main Data
 Name: Energy Out Value: 3.18966E+17
 OutQ [W] Signal: 0.00
 Delta P [Kpa] Range_Conversion [Fraction]: 0.9900

Material

PropName	In	Out
Is Recycle Part	<input type="checkbox"/>	<input type="checkbox"/>
Connected Stream/Unit Op	52/In	795/In
Temp [C]	374.3875	0.00
Pressure [Pa]	1000.001	1000.001
VolumeFlow [kg/mole/h]	300.0	300.0
MassFlow [kg/h]	644.96	601.85
VolumeFlow [m3/h]	28077.36	28077.48
ScaleVolumeFlow [m3/hr]	9260.719	21078.139
ScaleMassFlow [kg/hr]	42.536	34.646
ScaleVolumeFlow [SCMH]	4.8042E+5	3.4219E+5

Properties (All+):
 * Fraction [Fraction]
 * MassFraction [Fraction]
 * SdI/gfFraction [Fraction]
 * RoleFlow [kg/mole/h]
 * MassFlow [kg/h]
 * SdIqVolumeFlow [m3/hr]

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Carbonation reactor inlet flow specifications

ICON: Steam Gasification_latest - [Carbonation (ConvReactor)]
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Name: Carbonation Description:
 Type: Use Reaction Order Simultaneous Reaction

Summary Reactions Parameters Schematic

Run	
Run Name	Carbonation
Base Comp	CARBON DIOXIDE
Conversion (%)	99
Solution Order	D
CARBON MONOXIDE	
WATER	
CARBON DIOXIDE	-1
HYDROGEN	
METHANE	
CalciumOxide*	-1
CalciumCarbonate*	1
EP*	
OXYGEN	
Balance	5.00E-04
H ₂ (M ² /M ² S °C ³ /M ³)	3.11E+05

Carbonation: 1.0*CalciumCarbonate*-1.0*MCARBON_DIOXIDE-1.0*CalciumOxide*

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Carbonation reactor reaction specifications

Ready | iCON: Steam Gasification - latest - [Regeneration (ConvReactor)]

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Names | Regeneration | Description

Type: Use Reaction Order Simultaneous Reaction

Summary | Reactors | Parameters

Reactors	
Run Name	React
Regeneration	
Base Comp	CalciumCarbonate*
Conversion (%)	99
Solution Order	0
CARBON MONOXIDE	
WATER	
CARBON DIOXIDE	
HYDROGEN	
METHANE	
CalciumOxide*	1
CalciumCarbonate*	-1
EPB*	
OXYGEN	
Balance	-5.01E-07
Hydrogen (C) [kmol]	-3.11E+05

Regeneration: 10°C Calcium Oxide + 1, 10°C Calcium Oxide + 1, 10°C Calcium Carbonate*

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Regeneration reactor reaction specifications

Name	CO2_Disposal	CaO	CaO_Recycle	EFB	O2	Product_Gas	S1	S2	S3	S4	S5	S6	S7	S11	S12	Steam
VapFrac	1	0	0	0	1	1	1	0	1	0.5629	1	0	0	0	0	1
T [C]	950	950	950	150	950	950	950	140.7	950	149.9	950	950	950	950	950	150
P [kPa]	300	300	300	300	300	300	300	300	300	300	300	300	300	300	300	300
MoleFlow [kgmole/h]	242.3	250	250	100	350.49	435.75	845.23	375.39	260	375.39	600.49	492.3	250	595.23	60	
MassFlow [kg/h]	10663.46	14020	14127.71	9770	3199.88	3286.23	14057.4	28077.4	14054.99	14050.8	28077.53	24791.17	24791.29	14057.4	1080.92	
MassFraction.CARBON MONOXIDE	0	0	0	0	0.7358	0.0131	0.0861	0.0131	0	0.0132	0.0861	0	0	0	0.172	0
MassFraction.WATER	0	0	0	0	0.0265	0.1084	0.0031	0.0137	0.0769	0.0137	0.0031	0	0	0	0.0062	1
MassFraction.CARBON DIOXIDE	1	0	0	0	0.0331	0.774	0.3875	0.3905	0	0.3904	0.0039	0.4301	0	0	0.774	0
MassFraction.HYDROGEN	0	0	0	0	0.1556	0.0021	0.0182	0.0021	0	0.0021	0.0182	0	0	0	0.0364	0
MassFraction.METHANE	0	0	0	0	0.0094	0.0932	0.0011	0.0932	0	0.0932	0.0011	0	0	0	0.0022	0
MassFraction.CalciumOxide*	0	1	0.9827	0	0	0	0.4993	0	0	0	0	0.0105	0.56	0.0119	0	0
MassFraction.CalciumCarbonate*	0	0	0.0173	0	0	0	0	0	0	0	0	0.8725	0.0099	0.9881	0	0
MassFraction.EFB*	0	0	0	1	0	0.0397	0.0093	0.0046	0.2598	0.6953	0.2598	0.0046	0	0	0.0093	0
MassFraction.OXYGEN	0	0	0	0	1	0	0	0	0.2277	0.2277	0.2277	0	0	0	0	0

Mass balance table from iCON (T = 950°C, P = 300 kPa, Steam-to-Biomass ratio = 0.6)