

**Simulation of Gasification Technology on Multiple Feedstocks
Using ICON for Rich H₂ Production**

by

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**Dissertation submitted in partial fulfillment of
the requirements for the
Bachelor of Engineering (Hons)
(Chemical Engineering)**

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CERTIFICATION OF APPROVAL

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Approved by,

(Mr.Mohammad Tazli Azizan)

UNIVERSITI TEKNOLOGI PETRONAS

TRONOH, PERAK

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.

SURIA NORHANIYAA BT BASHRI

ABSTRACT

The use of hydrogen as an alternative fuel is gaining more acceptance as the environmental impact of hydrocarbons becomes obvious. There have many ways of alternative hydrogen production such as electrolysis, pyrolysis and gasification of biomass. Gasification coupled with gas shift is the most widely practiced process route for biomass to hydrogen. Thermal, steam and partial oxidation gasification technologies are under development around the world. The feedstocks may include agricultural and forest product residues of hard wood, soft wood and herbaceous species. However, the production efficiency (the amount of gaseous energy recovery from the feedstock used to produce hydrogen) must be improved and an infrastructure for efficiently transporting and distributing hydrogen is to be developed. This research project was carried out to simulate the gasification technology using multi feed stock basis where to find ways to obtain rich hydrogen gas. The raw materials that choosen as feedstock are empty fruit bunches, rice husk and rubber wood. The parameters that were investigated are reactor temperature is 900°C and steam/biomass ratio between 0.7-0.9 to obtain maximum hydrogen yield. The percentages of error of simulation compared to experimental data for hydrogen production is between 30% to 40%. Based on the comparison with experimental that done by Laohalidanond et.al (2006). At the end, the economic feasibility of the hydrogen production was investigated.

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CHAPTER 1

INTRODUCTION

1.1 Background of Study

The world's hydrocarbon resources are both limited and randomly distributed. All country faced the similar problems that are decreasing reserves of petroleum and natural gas. The only way to a future energy prices are affordable and relatively stable is to conserve energy, improve energy efficiency, and produce electric power, chemicals, fertilizers, and transportation fuels from plentiful (and thus relatively low-cost) domestic resources such as coal. (Hutchison, 2006)

Meanwhile, a whole new energy regime is being prepared. Hydrogen is the lightest and most abundant element in the universe and this is the next great energy revolution. Scientists call it the "forever fuel" because it never runs out and when hydrogen is used to produce power, the only byproducts are pure water and heat. Vehicles can be powered with hydrogen fuel cells, which are three times more efficient than a gasoline powered engine (Nath and Das, 2003). All these areas of hydrogen utilization are equivalent to 3% of the energy consumption, but it is expected to grow significantly in coming years.

According to Rifkin 2006,

"The hydrogen economy will make possible a vast redistribution of power, with far-reaching consequences for society. Today's centralized, top-down flow of energy, controlled by global oil companies and utilities, could become obsolete."

Hydrogen can be produced via various process technologies, including thermal (natural gas reforming, renewable liquid and bio-oil processing, and biomass gasification), electrolytic (water splitting using a variety of energy resources), and photolytic (splitting water using sunlight via biological and electrochemical materials).

Gasification is important because the syngas produced by this process could replace natural gas as the “fuel of choice” in the generation of electricity and literally help save many fertilizer and chemical industries. The capability of gasification to displace natural gas and petroleum is good enough to encourage extensive and rapid action of this proven technology.

1.2 Problem Statement

In very near future, it will be necessary to work intensively on the replacement of fossil fuels by high hydrogen content fuels. Production of hydrogen from renewable biomass has several advantages compared to fossil fuels. A number of processes are being practiced for efficient and economic conversion, and also utilization of biomass to hydrogen. Among all biomass conversion processes, gasification is one of the promising ones (Hussain et al., 2006). Gasification also is becoming one of the best clean technologies for power production (Nemtsov & Zabaniotou, 2008).

1.3 Objectives and Scope of Study

1.3.1 Objectives

The main objectives and the scope of study of this project are to simulate the gasification technology using multi feed stock basis. Then, this project also has to find ways to obtain rich hydrogen gas. Furthermore, there is a need to investigate the economic feasibility of this production.

1.3.2 Relevancy of the Project

The project is considered relevant to the current world energy situation. Over the last few years, interest in large scale biomass gasification has been growing steadily. Efficiency well over 40% has been predicted for such plants in the near future. For capacity range lower than 5-10 MW, new designs and catalytic gas cleaning may make a

new generation of biomass power gasifier feasible in the near future (Bhattacharya, 1997)

1.3.3 Feasibility of the Project within the Scope and Time Frame

This is a one year research project which includes the literature review, analytical analysis as well as modelling work. It is need to simulate the gasification technology using multi feed stock basis to obtain rich hydrogen gas. This project is considered to be feasible for execution throughout the required timeframe.

CHAPTER 2

LITERATURE REVIEW

2.1 World Energy Demand

Modern life depends upon energy and with each passing day it becomes more obvious that clean, climate-friendly, and affordable energy technologies must be set up as rapidly as possible. To that end, many countries are striving to make wind, solar, geothermal, hydrogen, and other “green” technologies as a larger part of their overall energy mix. However, for technical and economic reasons, it will be many decades before these resources can meet more than a fraction of the world’s energy demand. In the meantime, developed countries such as the United States and developing nations such as China and India will continue to rely upon hydrocarbons (natural gas, petroleum, and coal) for electricity generation and transportation fuel (Hutchison, 2006).

Natural gas that is clean-burning hydrocarbon is in great demand both as a fuel to heat homes and run power plants. Natural gas also used as a raw material for the manufacture of chemicals and fertilizer. As a result, a supply and demand imbalance exists in many other countries. Because of this imbalance, the price of natural gas is (and is projected to remain) too expensive for use in base load electric power plants or as a substitute for gasoline or diesel fuel.

Petroleum is also in high demand around the world and there is a corresponding supply and demand inconsistency. But even if the demand for petroleum were to decline or the supply to increase, we would not want for environmental reasons and to boost global consumption of gasoline, diesel, and other petroleum-based fuels. Also, like natural gas, petroleum is an important raw material for the production of chemicals and other high-value products. A strong case can be made that at least some of the world’s finite oil and gas resources ought to be conserved for such uses.

Coal is unlike oil and natural gas, coal is plentiful and inexpensive. The problem with coal is like one of the fundamental problems with petroleum that is the combustion

of coal creates air pollutants and carbon dioxide (CO₂). Although government and industry have cooperatively developed new “clean coal” technologies over the last three decades, there is still significant public opposition to the construction of coal-fired power plants. Such opposition arises because even the newest coal-fired plants emit criteria air pollutants (albeit at greatly reduced levels), airborne mercury, and millions of tons per year of CO₂ (which many scientists believe to be a major force in global climate-change).

2.2 Gasification Technology

Gasification is a flexible, reliable, and clean energy technology that can turn a variety of low-value feedstocks into high-value products. It is to help reduce our dependence on foreign oil and natural gas, and can provide a clean alternative source of baseload electricity, fertilizers, fuels, and chemicals. It is a manufacturing process that converts any material containing carbon such as coal, petroleum coke (petcoke), or biomass transferred into synthesis gas (syngas). Figure 2.1 shows the percentage of global syngas output by feedstock. The syngas can be burned to produce electricity or further processed to manufacture chemicals, fertilizers, liquid fuels, substitute natural gas (SNG), or hydrogen. Gasification has been reliably used on a commercial scale worldwide for more than 50 years in the refining, fertilizer, and chemical industries, and for more than 35 years in the electric power industry (Gasification Technologies Council, 2008).

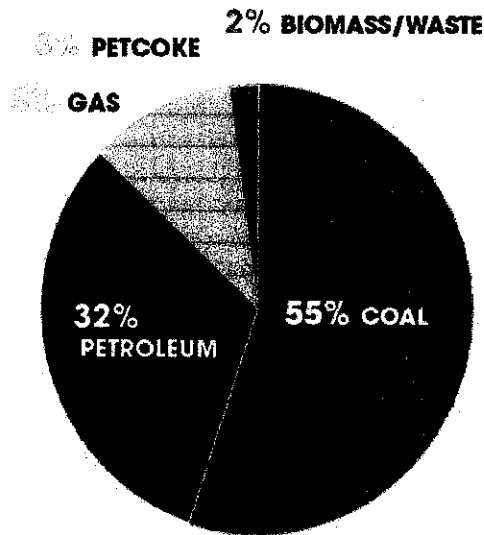


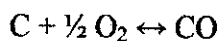
Figure 2.1: Global Syngas Output by Feedstock

[Source: Gasification Technologies Council 2008]

Gasification is a term that describes a chemical process by which carbonaceous (hydrocarbon) materials (coal, petroleum coke, biomass, etc.) are converted to a synthesis gas (syngas) by means of partial oxidation with air, oxygen, and/or steam. Modern gasification technologies generally operate in 3 steps. First, a hydrocarbon feedstock is fed into a high-pressure, high-temperature chemical reactor (gasifier) containing steam and a limited amount of oxygen. Second, under these “reducing” conditions, the chemical bonds in the feedstock are severed by the extreme heat and pressure and a syngas is formed. This syngas is primarily a mixture of hydrogen and carbon monoxide. Third, the syngas is then cleansed using commercially available and proven systems that remove particulates, sulfur, and trace metals (e.g. mercury). (Hutchison 2006)

Hydrogen can be extracted from biomass sources like wood chips and agricultural waste and be utilized as an energy carrier. Among the main reactions occurs in the gasifier are as follows (Higman & Burgt, 2003)

Partial oxidation

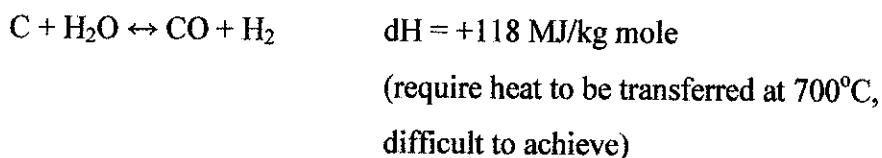


$$\text{dH} = -268 \text{ MJ/kg mole}$$

Complete oxidation



Water gas reaction

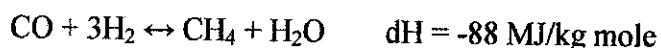


Carbon monoxide, hydrogen and steam can undergo further reactions during gasification:

Water gas shift reaction



Methane formation



For methane formation, high methane concentration is favored by low temperature and high pressure (Basu, 2006).

Three product gas qualities (in terms of calorific values (CV)) can be produced by varying the gasifying agent, method of operation and the process condition;

- | | | | |
|------|-----------|--------------------------|------------------------------------|
| i. | Low CV | 4-6 MJ/Nm ³ | Using air and steam |
| ii. | Medium CV | 12-18 MJ/Nm ³ | Using oxygen and steam (expensive) |
| iii. | High CV | 40MJ/Nm ³ | Using hydrogen via hydrogenation |

Low CV product gas can directly be used in combustion or as an engine fuel. Medium/high CV product gas can be utilized as feedstock for subsequent conversion into basic chemicals such as methane and methanol. Disadvantage of using air for gasification is that the nitrogen introduced along with the air dilutes the product gas, giving a net CV of 4-6 MJ/Nm³.

2.2.1 *Environment Aspect*

a) Gasification is an environmental solution

The world is facing rapid growth in energy demand, persistently high energy prices, and a challenge to reduce carbon dioxide emissions from power generation and manufacturing. No single technology or resource can solve the problem, but gasification can be part of the solution along with renewable power sources such as wind and energy efficiency programs.

Gasification can enhance the world energy portfolio while creating fewer air emissions, using less water and generating less waste than most traditional energy technologies. Whether used for power generation, for production of substitute natural gas, or for production of a large number of energy intensive products, gasification has significant environmental benefits over conventional technologies (Gasification Technologies Council, 2008).

b) Gasification provides significant environmental benefits

Gasification can reduce the environmental impact of waste disposal because it can use waste products as feedstock. It also generates valuable products from materials that would otherwise be disposed as wastes. Gasification's byproducts are non-hazardous and are readily marketable. Gasification plants use significantly less water than traditional coal-based power generation, and can be designed so they recycle their process water, discharging none into the surrounding environment. Gasification offers the cleanest, most efficient means of producing electricity from coal and the lowest cost option for capturing CO₂ from power generation.

2.2.2 Economic Aspect

Gasification can compete effectively in high-price energy environments to provide power and products. Gasification can be used to turn lower-priced feedstocks, such as petcoke and coal, into very valuable products like electricity, substitute natural gas, fuels, chemicals, and fertilizers. For example, a chemical plant can gasify petcoke or high sulfur coal instead of using high-priced natural gas, thereby reducing its operating costs.

While a gasification power plant is capital intensive (like any very large manufacturing plant), its operating costs are potentially lower than conventional processes or coal-fired plants. Gasification plants are more efficient and require less back-end pollution control equipment. With continued research and development efforts and commercial operating experience, the cost of these units will continue to decrease. Gasification offers wide fuel flexibility. A gasification plant can vary the mix of solid feedstocks, or run on gas or liquid feedstocks giving it more freedom to adjust to the price and availability of its feedstocks.

The ability to produce a number of high-value products at the same time (polygeneration) also helps a facility offset its capital and operating costs. In addition, the principal gasification byproducts (sulfur and slag) are readily marketable. For example, sulfur can be used as a fertilizer and slag can be used in roadbed construction or in roofing materials. Many predict that coal-based power plants and other manufacturing facilities will be required to capture and store CO₂, or participate in a carbon cap and trade market. In this scenario, gasification projects will have a cost advantage over conventional technologies. While CO₂ capture and sequestration will increase the cost of all forms of power generation, an IGCC plant can capture and compress CO₂ at one-half the cost of a traditional pulverized coal plant. This will provide a significant economic and environmental benefit in a carbon-constrained world. Gasification can replace increasingly expensive natural gas as a fuel or a feedstock (Gasification Technologies Council, 2008).

2.2.3 Future of Gasification

Worldwide gasification capacity is projected to grow 70 percent by 2015, with 80 percent of the growth occurring in Asia (refer to figure 2.2). The prime movers behind this expected growth are the chemical, fertilizer, and coal-to-liquids industries in China, oil sands in Canada, polygeneration (hydrogen and power or chemicals) and substitute natural gas in the United States, and refining in Europe.

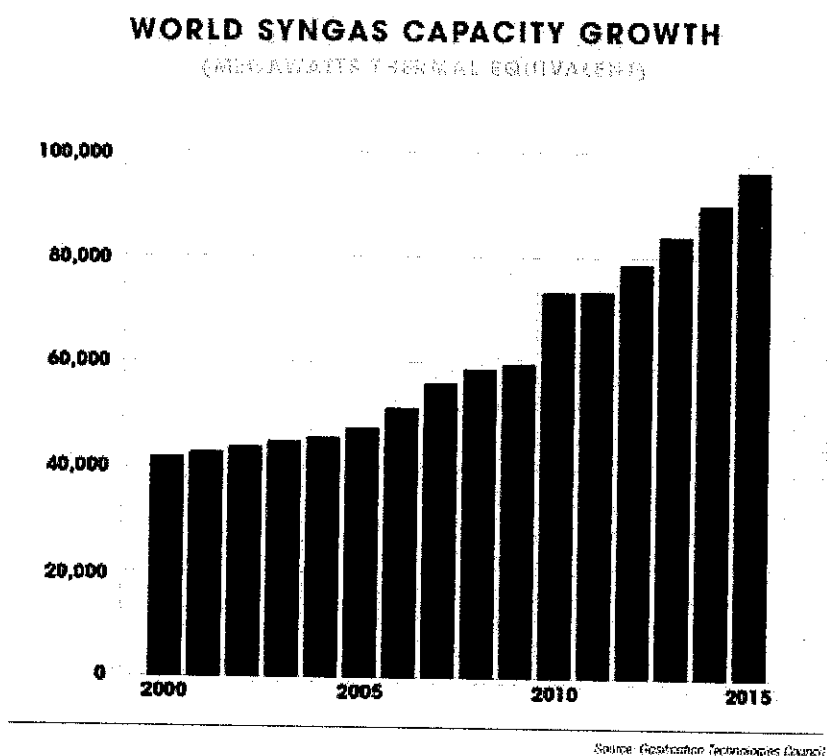


Figure 2.2: World Syngas Capacity Growth

[Source: Gasification Technologies Council 2008]

The use of gasification is expanding. Several gasification projects are under development to provide steam and hydrogen to upgrade synthetic crude in the oil sands industry in Canada. In addition, the paper industry is exploring how gasification can be used to make their operations more efficient and reduce waste streams. A number of factors contribute to a growing interest in gasification, including volatile oil and natural

gas prices, more stringent environmental regulations, and a growing consensus that CO₂ management will likely be required in power generation and energy production.

China is expected to achieve the most rapid growth in gasification worldwide. Since 2004, 29 new gasification plants have been licensed and/or built in China. In contrast, no new gasification plants have begun operation in the United States since 2002. The gasification industry is expected to grow significantly in the United States despite a number of challenges, including rising construction costs and uncertainty about policy incentives and regulations.

2.3 Simulation Software

2.3.1 *ICON Software*

According to Hashim and Chong (2007)

ICON is the PETRONAS own Process Simulation Software which is at par with commercial process simulators (e.g. HYSYS, UNISIM, PRO-2 etc.). It was launched in 2004 and has been widely used throughout PETRONAS OPU's. ICON open architecture and built-in linkage with Microsoft products makes it suitable to be connected to PI (Plant Information) for online monitoring and optimization purposes.

According to Lee, (2003-2007)

ICON is a state of the art steady-state process simulator constructed using the most advanced off-the-shelf technology for reliability, convenience and cost. ICON itself is a graphical user interface (GUI) that includes all the facilities one expects from a chemical process simulator such as unit operation forms, graphs, unit conversion and process flow diagrams. In addition, ICON provides a powerful Excel unit operation that allows you to embed Microsoft Excel spreadsheets directly into the flowsheet. ICON uses VMGSim as the process simulation kernel. VMGSim is an advanced process simulator produced by Virtual Materials Group Inc. This process simulation kernel is written in the Python programming language and extremely flexible, supporting

bidirectional information flow, partial information propagation and a comprehensive set of unit operations. Finally, ICON uses VMGThermo as the engine for thermodynamic and physical property calculations. VMGThermo is an advanced physical property calculation system that includes all necessary property packages for natural gas, refinery, petrochemical and chemical processing simulation, together with a rigorous multiphase flash system.

According to *Simulation Application in Thermodynamic* (2006)

ICON is based squarely on fundamental thermodynamic principles. These principles are used in two main features of the process simulator that are the thermodynamic calculation engine and the simulation solver for unit operation and flowsheet. The thermodynamic engine provides rigorous thermodynamic equilibrium and physical property estimation for industrially important systems. The simulator solver continually monitors the degrees of freedom of the flow sheet. It will immediately invoke the necessary calculations when the degrees of freedom are complete. It also solved the system of equations describing the flow sheet.

2.3.2 Hysys Software

According to *HYSYS Integrated Engineering Environment* 1997,

HYSYS is the process simulation software for the chemical, petrochemical and hydrocarbon processing industries. HYSYS Integrated Engineering Environment (conceptual design, steady state, dynamics, DCS Checkout, operator training, on-line optimization, empirical modeling, etc.)

HYSYS facilitates software integration by providing engineers access to a wider range of technologies in a single modeling environment. With HYSYS, you only need to develop one simulation model and then select the appropriate simulation solver: conceptual design, steady state, dynamics, etc. HYSYS models can even be linked to plant hardware to support real-time applications such as DCS checkout, operator training and online optimization. At the core of HYSYS is the common

information which is shared by the various simulation solvers: a solid thermodynamics foundation, a wide range of property packages, an extensive component database and a comprehensive selection of unit operations. Modifications to any of this common information are immediately available to all simulation solvers.

Additionally, due to its advanced object-oriented structure and full OLE compliance, HYSYS can send and receive information from other applications such as MATLAB, Excel, Word or Visual Basic. This enables users to create custom applications that access the power of HYSYS or build custom front-ends that allow access only to certain parts of the simulation from a custom-designed interface. Furthermore, HYSYS allows the seamless integration of custom unit operations, reaction kinetics and property packages that can be created from scratch or from legacy Fortran or C code. HYSYS offers an optional OLE/DDE interface to MATLAB so that its sophisticated features can be used in conjunction with the advanced process modeling capabilities of HYSYS. For example, MATLAB can be used to simulate advanced process control schemes during dynamic simulation.

Application Areas:

- Control system design/analysis
- Data analysis/modeling
- Manufacturing
- Petrochemical
- Process control/monitoring
- Simulation

2.4 Simulation of Gasification

Several simulation of gasification has been done earlier using Aspen Plus simulation software. (Shen et.al(2007), Nikoo & Mahinpey(2007) etc.)

2.4.1 Interconnected Fluidized Bed Simulation

A possible design for hydrogen production from biomass catalytic gasification is the interconnected fluidized beds that have been studied by Shen et al. (2007). They use ASPEN PLUS simulation software and steam as gasification agent. 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.

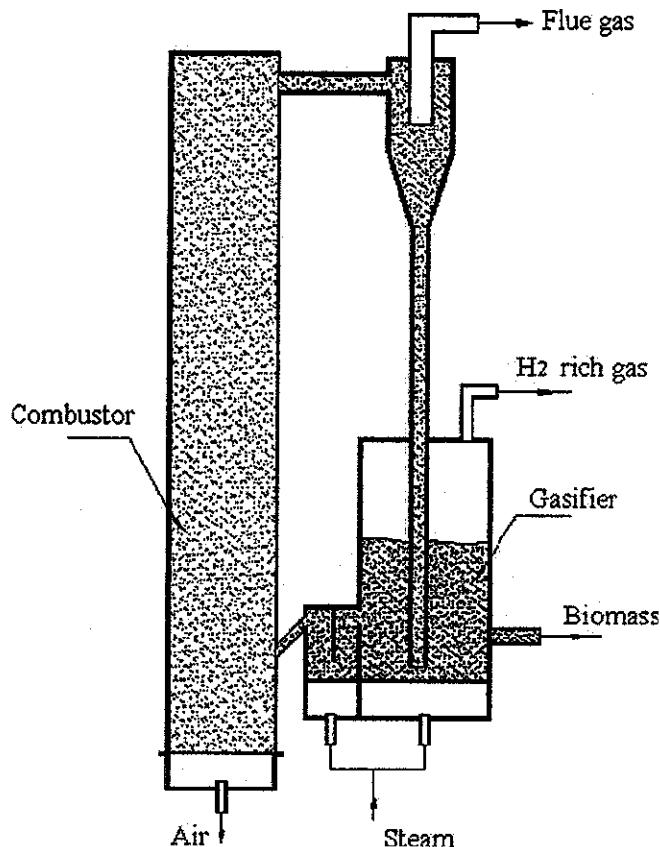


Figure 2.3 Scheme of biomass gasification in interconnected fluidized beds

The design of interconnected fluidized beds is shown in Figure 2.3. It is a loop with end-to-end configuration. The figure resembles a circulating fluidized bed with the extra bubbling fluidized bed after the cyclone. The circulating fluidized bed is designed for combustion fed with air, the bubbling fluidized bed for biomass gasification fed with steam.

The flow chart of simulation for biomass gasification in interconnected fluidized beds is sketched in Figure 2.4. The whole model consists of two basic modules, a gasification module and a combustion module. The gasification module is composed of a pyrolyzer and a gasifier. The pyrolyzer block is merely a decomposer, which corresponds to Ryield block of Aspen plus; its function is to decompose biomass into simple components. The operating conditions and primary parameters in the simulations were illustrated in Table 2.2.

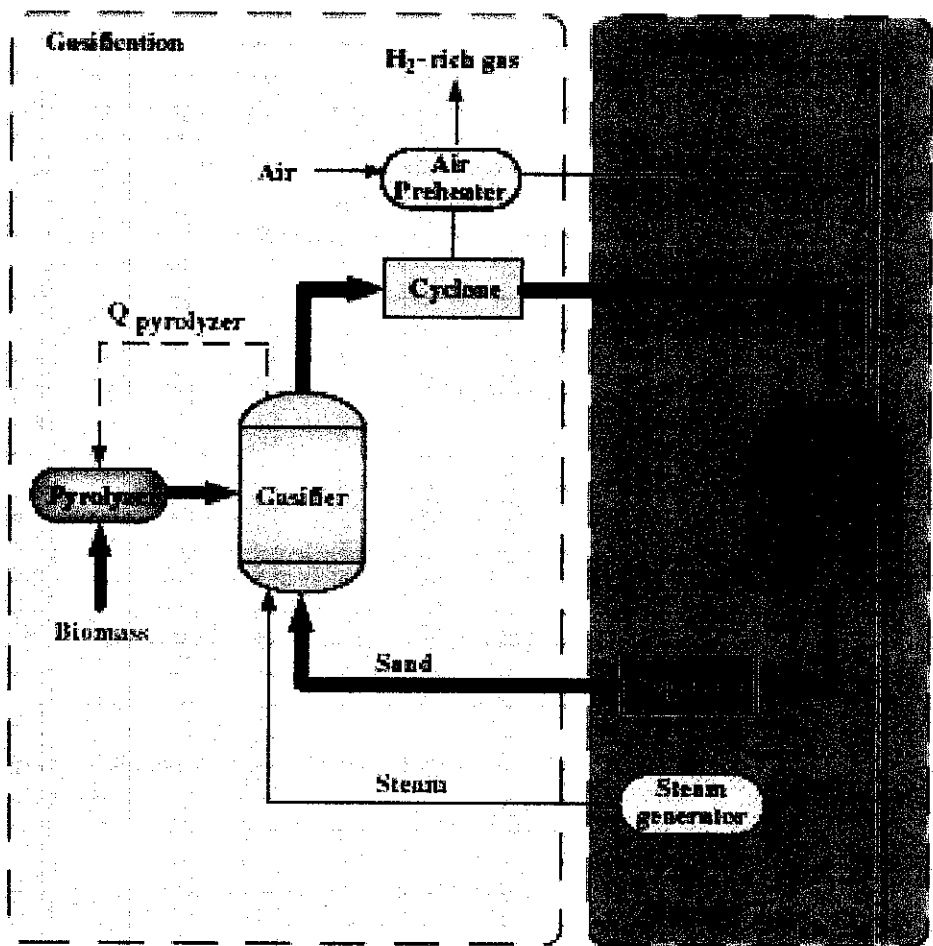


Figure 2.4: Simulation of Biomass Gasification in Interconnected Fluidized Beds

Table 2.1 Parameters in Interconnected Fluidized Bed Simulation

Room temperature	20°C
Biomass flow rate	1 kg/s
Air flow rate	2 kg/s
Steam temperature (generated in steam generator)	600°C
H ₂ -rich gas (after the air preheated)	500°C
Combustor temperature	900-950°C
Gasifier temperature	650-900°C
System pressure	0.1 MPa

The results that obtained from the paper are the hydrogen yield will be maximum at gasifier temperature between 750 °C to 800°C, the combustor temperature should be at 920 °C. Higher temperature favors the reactants in exothermic reactions and favors the products in endothermic reactions. Therefore, endothermic reactions (steam gasification, boudouard, steam reforming) were strengthened with an increase in the gasifier temperature, which resulted in an increase of H₂ and CO and decrease of CO₂ and CH₄. The value of steam/biomass ratio is between 0.6 to 0.7. This was explained by the chemical equilibrium of the water-gas shift reaction. The increase of steam meant that the higher concentration of reactants would promote the reactions (steam gasification and water-gas shift) towards the right direction (the reactions were favored). Optimum hydrogen yield that obtained from this paper is 54-62g H₂/kg biomass. Hydrogen and carbon dioxide contents increase smoothly with the increase of the steam/biomass ratio, while carbon monoxide content dropped continuously. The increment of hydrogen yield was distinct with the increase of the steam/biomass ratio at lower gasifier temperature (below 750 °C).

2.4.2 Atmospheric Fluidized Bed Simulation

Other simulation of biomass gasification using ASPEN PLUS software has been done by Nikoo and Mahinpey (2007). The gasification equipment and gasification agent that they use is fluidized bed reactor and steam. They present the details of the modeling approaches taken to obtain a process simulation program for biomass gasification in a fluidized bed reactor. 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 following assumptions were made in simulating the hydrodynamics;

- a) Fluidized reactor is divided into 2 regions (bed and freeboard).
- b) The fluidization state in the bed is maintained in the bubbling regime.
- c) The volume fraction of solids decreases as height increases.
- d) Volumetric flow rate of gas increases along with height.
- e) The mixing of ash, char particles and bed material.
- f) The reactor is divided into a finite number of equal elements with constant hydrodynamic parameters.
- g) The fluidized bed is one-dimensional (variations only occur in the axial direction).

A comprehensive simulation diagram for the fluidized bed gasification system is given in Figure 2.5. The experimental setup parameters used in the simulation were illustrated in Table 2.2.

Table 2.2 Parameters in Atmospheric Fluidized Bed Simulation

Reactor temperature	700-900°C
Reactor pressure	1.05 bar
Bed diameter	40 mm
Freeboard diameter	60 mm
Reactor height	1400 mm
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
Silica sand average particle size	0.275mm
Silica sand weight	30g

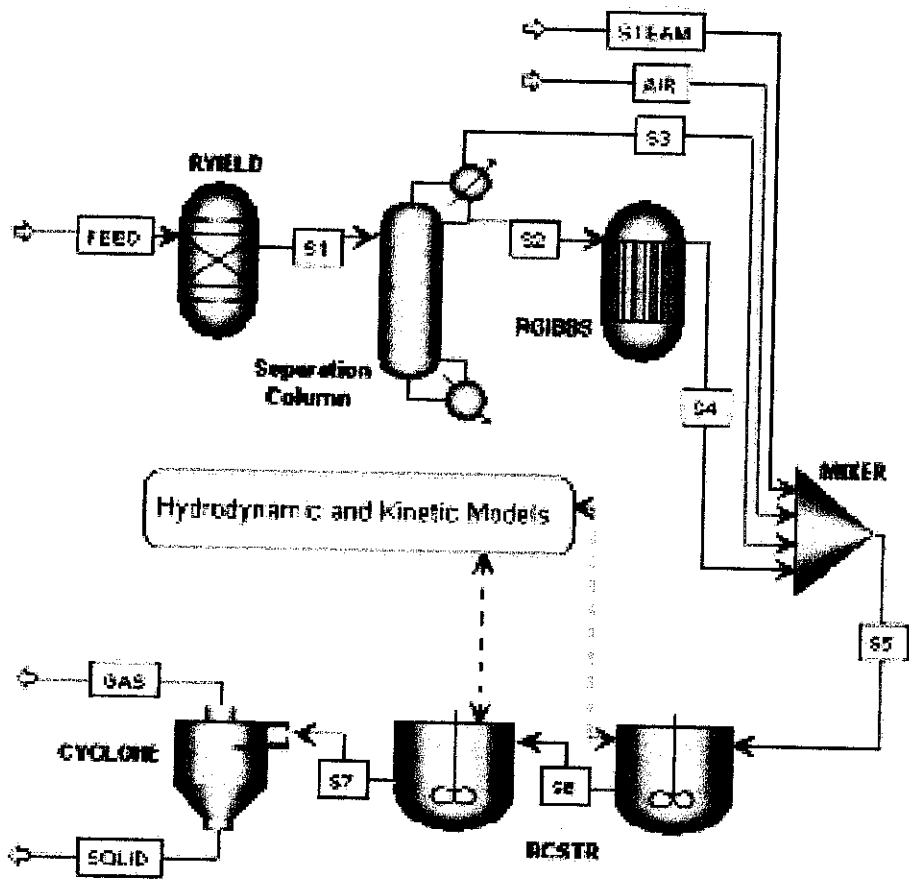


Figure 2.5: Simulation Diagram for the Fluidized Bed Gasification System

Hydrogen composition that obtained in this research paper are around 40-50 mol% and the highest hydrogen composition is at 900°C of reactor temperature. Increasing in reactor temperature had decreased the composition of carbon monoxide and methane but the composition of carbon dioxide showed contrast trend. Biomass produces more tar and unburned hydrocarbon in lower temperature, which decreases hydrogen production. Corresponding to steam gasification reaction, the higher amount of hydrogen favors the backward reaction. Furthermore, the backward reaction (steam gasification) dominates the prediction of carbon monoxide and it shows slight underestimation in temperatures lower than 800°C. Hydrogen composition increases when the steam/biomass ratio increases. The percentage of hydrogen in product gas is the best precision for gasification without steam because of the low amount of tar in the process. Higher flow rate of steam decreases carbon monoxide and increases carbon dioxide in the product gas.

2.5 Experimental of Gasification

Experimental on gasification has been done by Lv et al. (2002). The tests were performed in an atmospheric pressure, indirectly heated, fluidized-bed gasification system, which is shown schematically in Figure 2.6. Its major components are the fluidized-bed gasifier, biomass feeding system, steam and air providing and preheating system, gas metering, cleaning and sampling system, temperature control system, and gas off-line analysis system.

Below the reactor, one air distributor was installed for better air distribution. The biomass was fed into the reactor through one screw feeder driven by a variable speed metering motor. The air was used as the fluidizing agent and came from the air compressor. Before the air entered into the reactor, it was preheated to 65 °C in the preheater for better performance. The steam of 154 °C was produced in a steam generator. The produced gas flow exits the reactor, and then passes through a cyclone, which is heated to 200 °C to prevent the tar contained in the gas condensing in it. Then the two electric furnaces were turned on to preheat the fluidized-bed reactor; meanwhile, the air preheater was turned on.

In the interval of reactor preheating, the steam was prepared for the test. After the bed temperature reached the desired level and was kept steady, the air compressor was turned on to force the air through the preheater, air distributor, and into the reactor. When the bed temperature again turned steady, the screw feeder was turned on at the desired rotate speed and the test began. The feedstock that been using in this experimental work is pine sawdust.

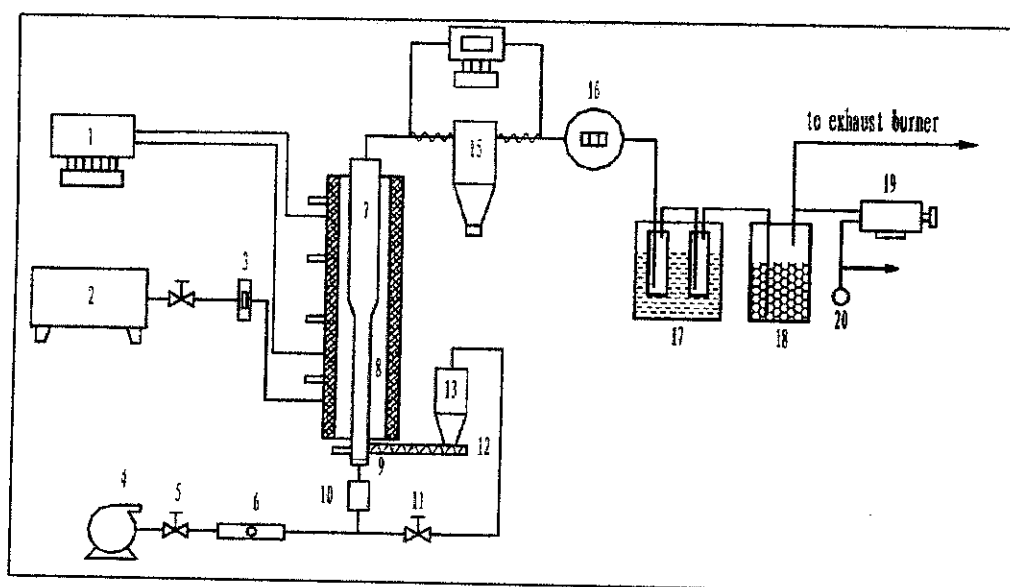


Figure 2.6: Schematic Diagram Of Biomass Air-Steam Gasification In A Fluidized Bed.

From the experimental result, the higher reactor temperature, proper steam/biomass ratio and smaller biomass particle size will contribute to more hydrogen production. The highest hydrogen yield is 71g H₂/kg biomass (wet basis) was achieved at a reactor temperature of 900°C. According to Lv et al. (2002), under proper operating parameters biomass air-steam gasification in a fluidized bed is one effective way for hydrogen-rich production.

2.6 Feedstocks

2.6.1 Biomass

Biomass was the world's first fuel and source of energy, but when coal became widely available, to be followed later by bio-oil and natural gas, its use declined (Hussain et. al, 2006). However, in recent years interest in it has been renewed, much of being focused on its efficient conversion for energy.

The agriculture biomass has a higher hemicellulose and protein content, but lower lignin content. The lower amount of lignin content (15-25%) shows that the substances have very high energy content (Scahill, 2003). Agricultural biofuels are less aromatic compared to the woody biomass with functional groups that are more oriented towards hydroxyl, with lower concentrations of methoxyl (lower amount of lignin).

Depending on the raw material in use, the conversion of lignocelluloses wastes or more generally of dry biomass can be achieved after reducing the feedstock to a suitable particle size distribution by grinding, by partial oxidation or by flash pyrolysis. Biomass that have dry matter content over 70wt% to 80wt% as opposed to "wet" agricultural wastes which are used for fermentation.

Biomass conversion could be classified into two type; biological and non-biological process. The biological processes included anaerobic methane formation and the ethanol fermentation production. The non-biological processes are mainly the ones involve thermal processes such as combustion (with excess air), pyrolysis (with no air or oxygen present), and gasification (with partial air).

2.6.2 Properties of Feedstocks

Raw materials that can be used as feedstock are empty fruit bunches (EFB), rice husk and rubber wood. The proximate analysis and the ultimate analysis of the raw materials were illustrated in Table 2.3:-

Table 2.3 Proximate and Elemental Analysis of Biomass Feedstock

	Empty Fruit Bunches (Hussain et.al,2006)	Rice Husk (Laohalidanond et.al., 2006)	Rubber Wood (Srinivasakannan & Zailani,2003)
Proximate analysis (wt%)			
Moisture	6.8	8.20	6.2
Volatile	77.4	58.90	69.68
Fixed C	19.3	19.70	23.38
Ash	3.3	13.20	0.74
Elemental analysis (wt%)			
C	49.5	39.10	43.98
H	5.9	4.59	8.04
N	0.5	0.18	0.14
O	40.6	34.70	47.53

2.6.3 Effect of Feed Properties on Gasification

The following section describes the effect of feed properties on the composition of the product gases.

2.6.3.1 Reactivity

Physical properties such as particle size have significant effects in the kinetics of gasification. As the particle size becomes smaller, the specific contact area between the particle and the reaction gases increases, resulting in faster reactions.

2.6.3.2 Volatile Matter

On a dry basis, the volatile matter content of a fuel varies from less than 5% in the case of anthracite to more than 75% in the case of wood. The reactivity and conversion to char inside the gasifier depend on its volatile matter content. Feed

with higher volatile matter content are more reactive and therefore can be converted more easily to gas, producing less char.

Biomass feedstock, such as wood, is highly reactive and characterized by high volatility content. Thus, these fuels produce relatively small amounts (~25% of the weight of the original dry fuel) of char and the char also more porous and react relatively fast. For this reason, fuels with high volatile matter content are easier to gasify. However they produce gas with a high tar content, which makes gas clean-up more difficult. (Basu, 2006)

2.6.3.3 Ash

The ash content does not have much direct influence on the composition of the product gases, but the practical operation of the gasifier will be affected. For example, in a gasifier operation, ash is an avoidable nuisance that has to be separated from the product gases and suitably disposed of. Depending on the design, the ash is removed in either solid or liquid form from a gasifier.

2.6.3.4 Moisture

The moisture content of wood from a freshly harvested tree is typically around 50%. High moisture content of feed lowers the temperature inside the gasifier since evaporation as well as the chemical reaction of steam with char is endothermic. Therefore, an upper limit of moisture content is set for satisfactory gasification. For example, in a typical fixed bed this limit is about 35% for a good quality coal (moderate rank and ash content), and about 25% for wood. Fluidized and entrained bed gasifier, with their lower tolerance of moisture content normally require moisture content of the feedstock to be reduced to 5% to 10% (Basu, 2006).

2.6.3.5 Density

The density will determine the net energy content of a biomass feedstock. Density varies within and between species. For example, wood from young trees is less dense than from old trees of the same species, and sapwood is less dense than heartwood. Various techniques are also used to make biomass feedstocks

denser in order to reduce transport costs and to make them more manageable. The density of wood can vary from as low as 150 kg/m^3 to over 600 kg/m^3 as stacked logs. (Calle et. al, 2007)

CHAPTER 3

METHODOLOGY

The estimated work flow throughout this project is summarized in the schematic flow diagram as shown below:

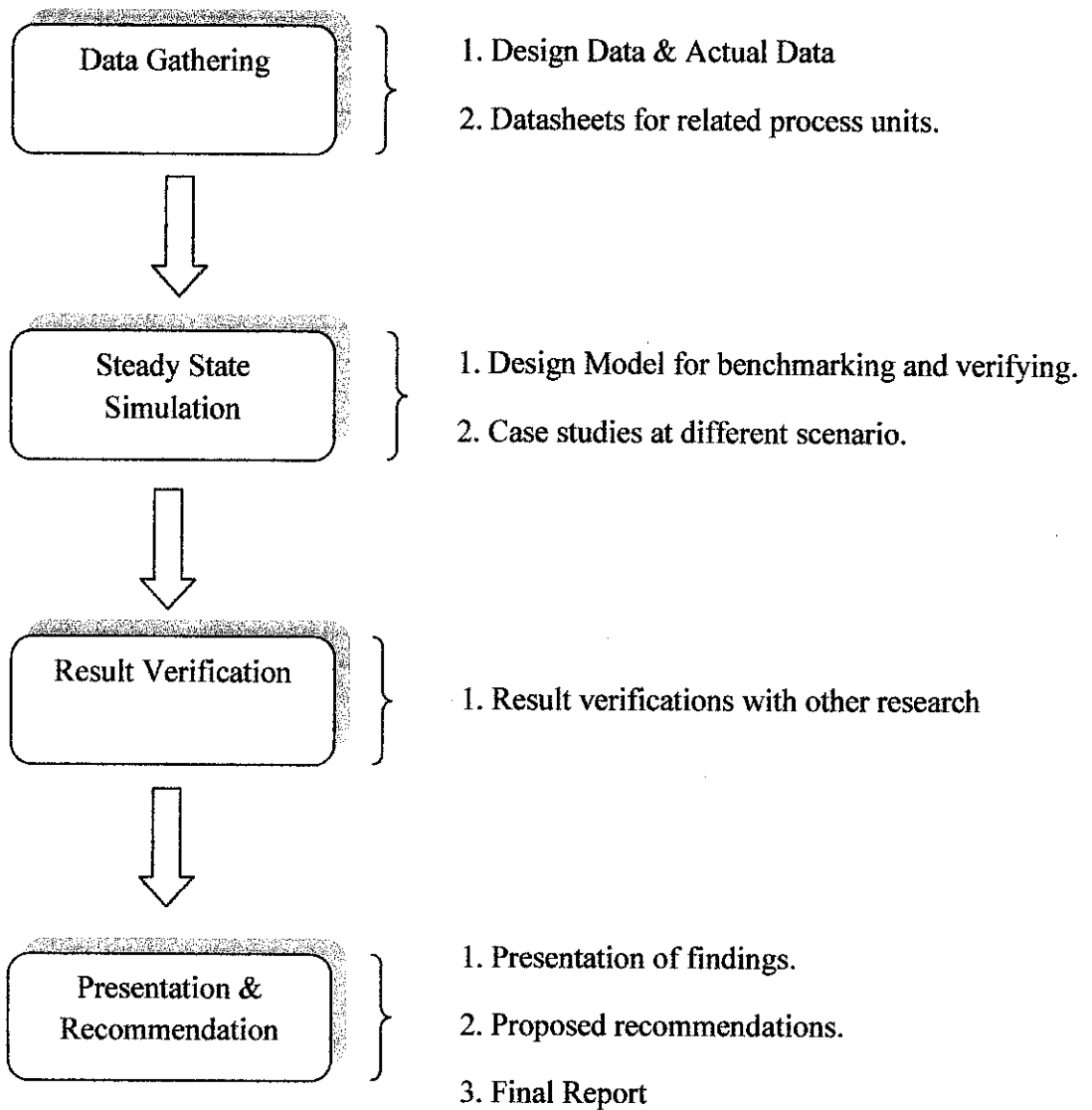


Figure 3.1: Schematic flow of project

3.1 Gasification Methods

Among the proven combustion technologies such as grate-fired systems and suspension-fired systems, the fluidized bed is reported to be most efficient and suitable for converting agricultural and wood residues into energy (Bridgewater, 1994). Before gasification is conducted, the feedstock has to be pre-treated for its moisture content, particle size as well as the nitrogen and alkali contents of the biomass. The biomass moisture content should be below 10-15% before gasification. Feedstock particle sizes in the range of 20-80 mm are typical. Small particles tend to contain less nitrogen and alkali, so fractionation into fine and coarse particles helps to produce gas with fewer impurities. The nitrogen and alkali content can be reduced via leaching with water.

In the processes of hydrogen production from biomass catalytic gasification, the bubbling fluidized bed gasifier is at a temperature range of 650–900 °C. As soon as biomass is fed into the bottom of the bubbling fluidized bed, an exquisite contact between biomass and hot bed particles occurs, followed by the intense exchange of heat and mass.

The overall process of biomass gasification in the bubbling fluidized bed can be divided into four steps. The first step is drying, where the moisture of biomass evaporates. The second step where volatile compounds in biomass evaporate is called devolatilization. This is followed by the step where the major part of the carbon content of biomass is converted into gaseous compounds. The result is, apart from gases, a carbon-rich solid residue called char. In the last step, the char is partly gasified with steam and converted into gaseous products. The amount of unreacted char is a function of gasification conditions, such as temperature and biomass particle residence time in the gasifier. The gas stream from the bubbling fluidized bed consists of a mixture of hydrogen, carbon monoxide, carbon oxide and a small amount of methane and tar (Shen et.al,2007).

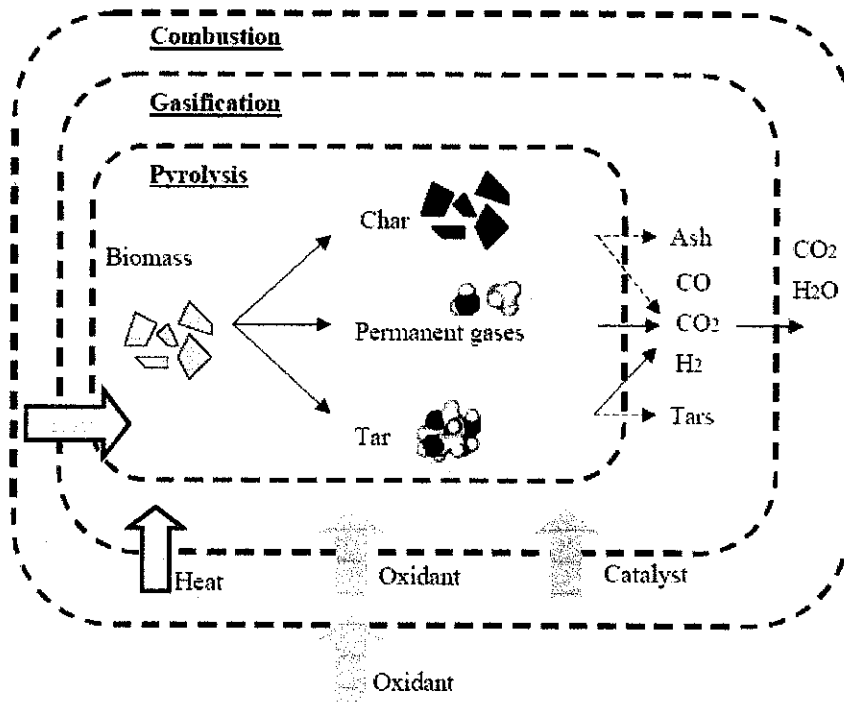


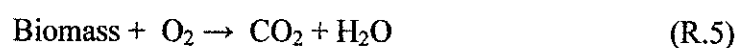
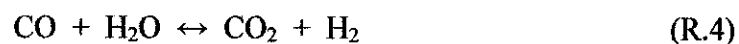
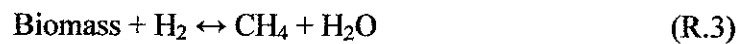
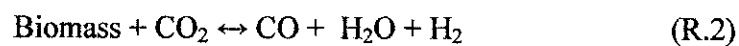
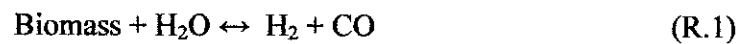
Figure 3.2: Block Diagram for the Gasification Process Flow

(Source: BTG Biomass Technology Group BV, 2009)

3.2 Setup Parameters

3.2.1 Reactions in Reactor

The main reactions involved in the process are given below:-



The flow chart of simulation for biomass gasification in interconnected fluidized beds is sketched in Figure 3.3. Where, the reactions that occurred in R-1 (reactor 1) are steam gasification (R.1), Boudouard (R.2) and methanation (R.3). Then, water-gas shift reaction (R.4) occurred in R-2 (reactor 2). Products from R-2 are sent to combustor, R-3 and react with oxygen for combustion reaction (R.5). Finally, steam reforming reaction (R.6) takes place in R-4 (reactor 4). The equilibrium constants for some of the above chemical reactions are tabulated below in Table 3.1:

Table 3.1: Kinetic coefficients of gasification reactions

Reactions	$K_{0,i}$	$\Delta\tilde{G}_{0,i} / \tilde{R} \text{ (K)}$	References
R.1	3.139×10^{12}	16344	(Hottel et al., 1971)
R.2	1.238×10^{10}	20294	(Parent et al., 1948)
R.3	1.435×10^{11}	-11005	(Hottel et al., 1971)

Where

$\Delta\tilde{G}_{0,i}$ = 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)

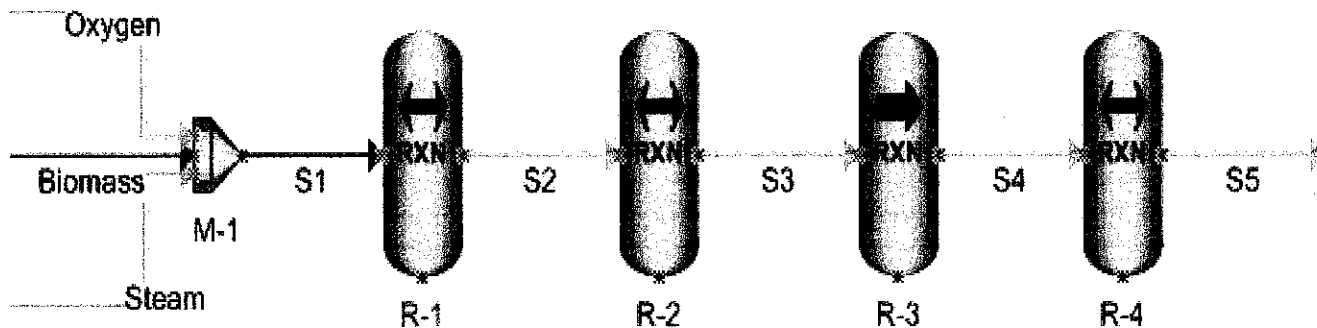


Figure 3.3: Simulation Diagram of Gasification using ICON Software

3.2.2 Parameters

Table 3.2: Parameters Setup in iCON Simulation

Room temperature	20°C
Biomass flow rate	75 kg/hr
Oxygen flow rate	10.5 kg/hr
Steam temperature	600°C
Combustor temperature	900-950°C
Gasifier temperature	650-900°C
System pressure	100 kPa
Steam/biomass ratio	0.4-0.9

3.2.3 Feedstocks

In ICON simulation software, biomass feedstock was consider as hypothetical compound. Thus, several data need to be included in the hypothetical compound such as molecular weight and density of the compound.

Table 3.3: Multiple Feedstocks

Feedstock	Empty Fruit Bunches	Rice Husk	Rubber Wood
Chemical Formula	$C_{3.4} H_{4.1} O_{3.3}$	$C_{4.1} H_{5.8} O_{2.8}$	$C_4 H_6 O_{2.4}$
Molecular Weight (kg/kgmole)	97.7	99.8	92.4
Density (kg/m ³)	450	1063	626

Details in reaction that occur in every reactor for each feedstock were attached in the appendices.

CHAPTER 4

RESULTS AND DISCUSSION

4.1 Effects of Reactor Temperature

It is known that temperature plays an important role in biomass gasification. In the present work, the reactor temperature was increased from 650 °C to 900°C in 50°C increments to investigate the effect of temperature on gas composition and hydrogen yield and the results referring only to steam/biomass ratio of 0.6. The simulation results are presented in figure below:

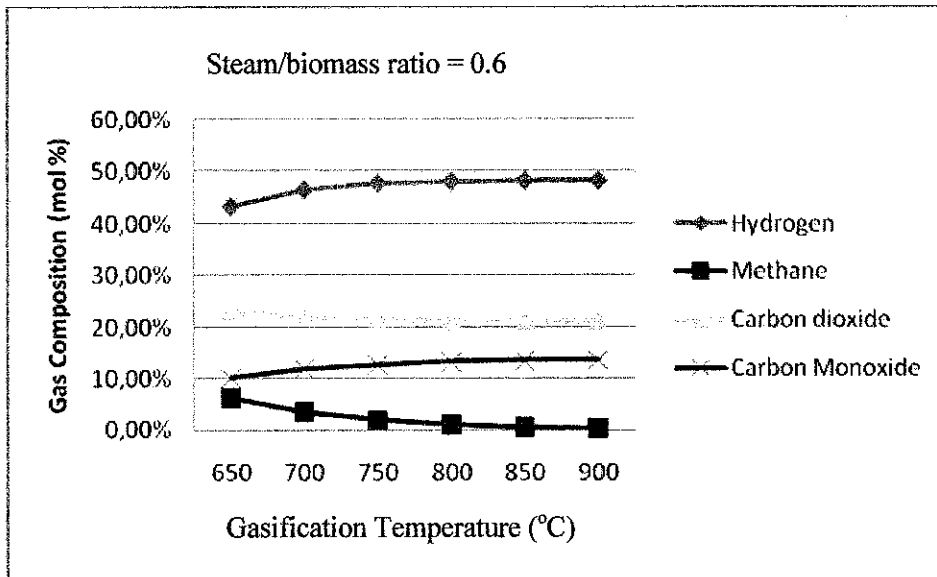


Figure 4.1: Effect of Gasification Temperature on Gas Composition of Empty Fruit Bunches (EFB)

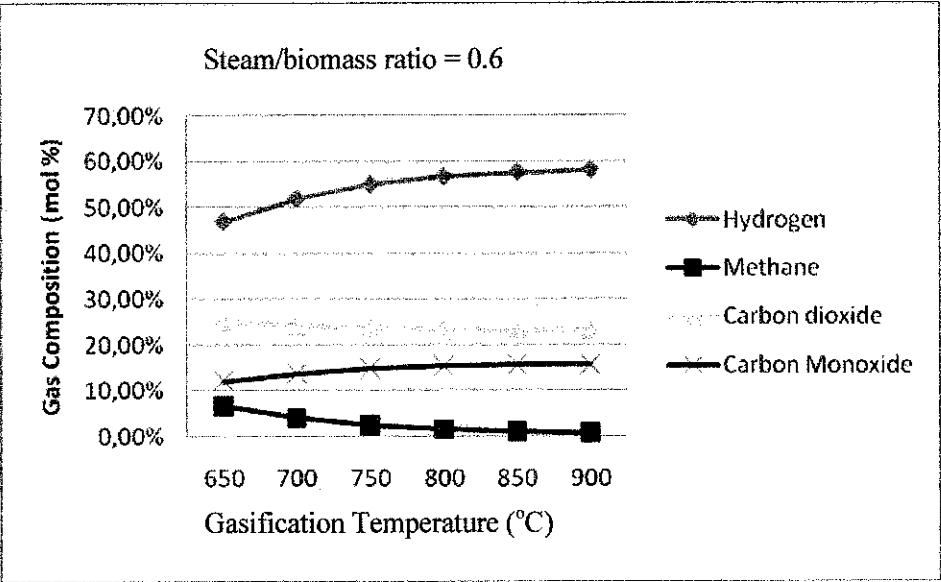


Figure 4.2: Effect of Gasification Temperature on Gas Composition of Rice Husk

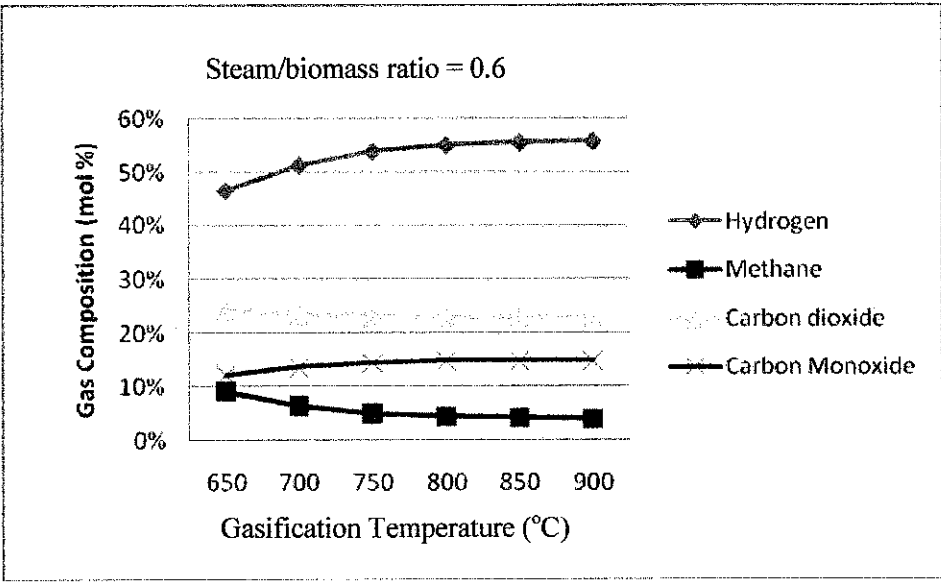


Figure 4.3: Effect of Gasification Temperature on Gas Composition of Rubber Wood

The gas composition is shown as a function of the gasifier temperature. The Hydrogen content was maintained around 40-60 mol% for every feedstocks at the temperature range of 650-900°C. Research done by Shen et al. (2007) also gets the similar result. The gas yields increase with the increase in reactor temperature, whereas according to experimental result, the tar and char yields decrease. (Wei et al., 2006)

Higher temperatures favor the reactants in exothermic reactions and favor the products in endothermic reactions. Therefore, endothermic reactions (steam gasification, boudouard and steam reforming) were strengthened with the increasing temperature in the gasifier which resulted in increase in of Hydrogen and Carbon Monoxide and decrease of Carbon Dioxide and Methane (Shen et al. 2007). At the same time, water-gas shift reaction greatly determines the dry gas composition, which contributes to the increase in Hydrogen production. The Methane content in the dry gas slightly decreases inferred that Methane reforming is still difficult, even in elevated temperatures under experimental conditions (Wei et al. 2006). These results can be referred to Figure 4.1, Figure 4.2 and Figure 4.3. The trend of gas composition were similar for empty fruit bunches (EFB), rice husk and rubber wood.

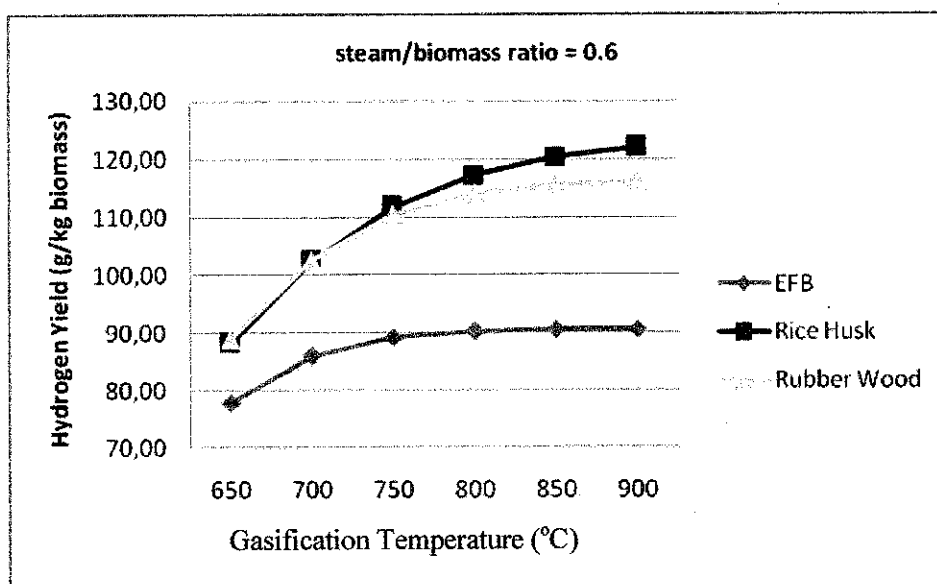


Figure 4.4: Effect of Gasification Temperature on Hydrogen Yield (g/kg biomass) at Different Feedstocks

In Figure 4.4, it can be observed that rice husk showed higher hydrogen yield (g/kg biomass) while the empty fruit bunches is quite low. It might be attributed to the variant chemical components of different biomass samples, because rice husk showed higher volatile component and Hydrogen content compared to empty fruit bunches where it showed lowest volatile component and Hydrogen content (Hanping et al., 2008).

4.2 Effects of Steam/Biomass Ratio

The effects of the steam/biomass ratio on hydrogen production from biomass gasification were also studied. The steam/biomass ratio was varied by changing the steam flow while keeping the biomass flow constant. The effect of the steam/biomass ratio on gas composition at the gasifier temperature of 900°C is shown in figure below:

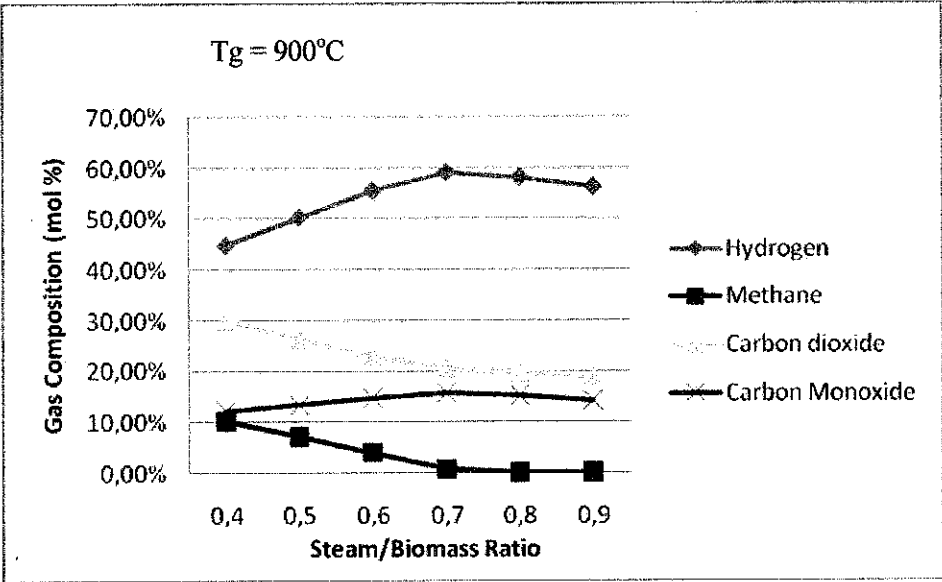


Figure 4.5: Effect of Steam/Biomass Ratio on Gas Composition of Empty Fruit Bunches

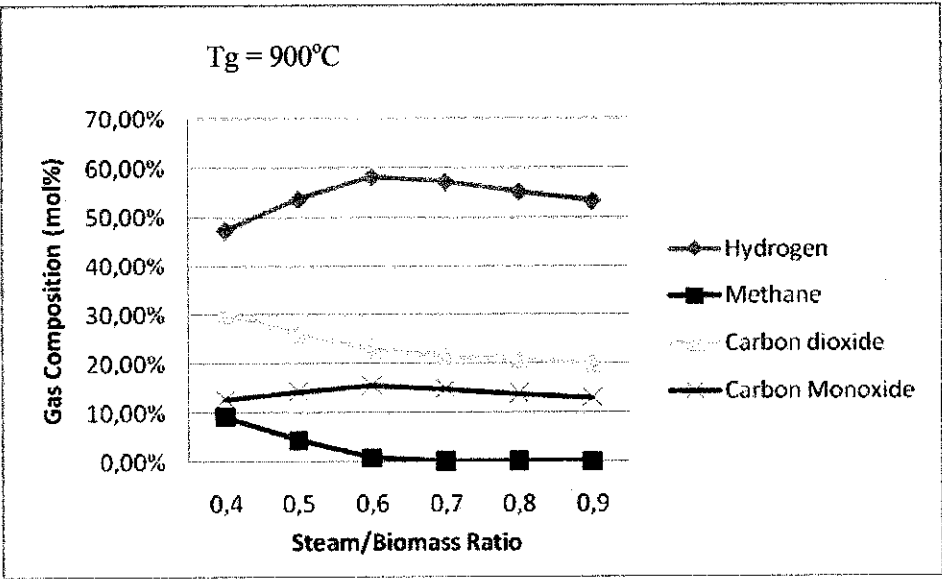


Figure 4.6: Effect of Steam/Biomass Ratio on Gas Composition of Rice Husk

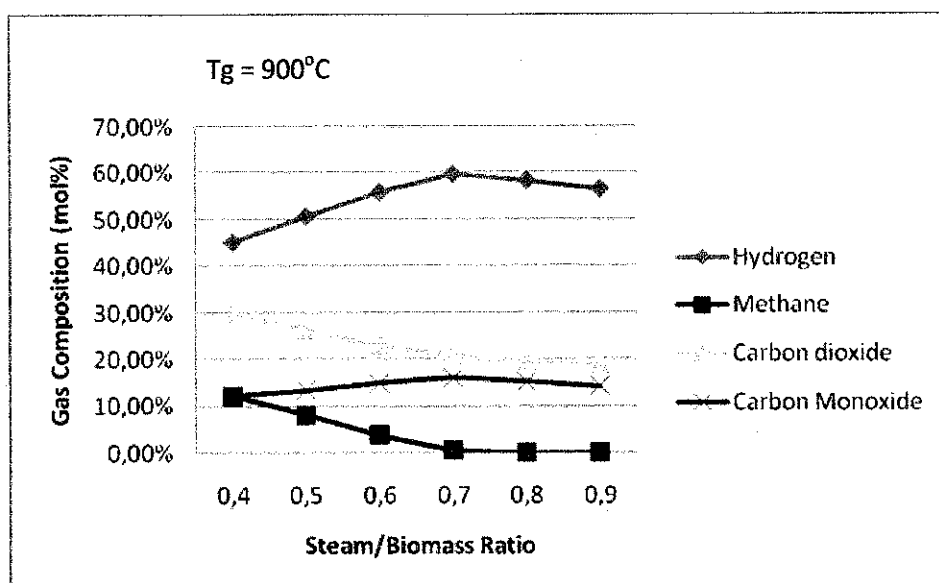


Figure 4.7: Effect of Steam/Biomass Ratio on Gas Composition of Rubber Wood

As shown in Figure 4.5, Figure 4.6 and Figure 4.7, it is found that hydrogen and carbon monoxide composition increase with an increase in the steam/biomass ratio from 0.4 to 0.7 whereas the carbon monoxide and methane composition decreases. It shows that, the addition of steam favors hydrogen formation. While, the hydrogen/carbon dioxide molar ratio increases with an increase in the steam/biomass ratio. It can be inferred that the steam reforming reaction plays an important role in determining the dry gas composition and hydrogen production.

The results seem to suggest that steam/biomass ratio of about 0.6-0.7 should be selected for further work. For steam/biomass ratios lower than 0.6, there was not enough steam to react with the biomass, consequently steam gasification reaction (R.1), water-gas shift reaction (R.4) and steam reforming reaction (R.6) did not appear to reach a state of completion. As a result, hydrogen composition increased with the rise of the steam/biomass ratio (Shen et al., 2007).

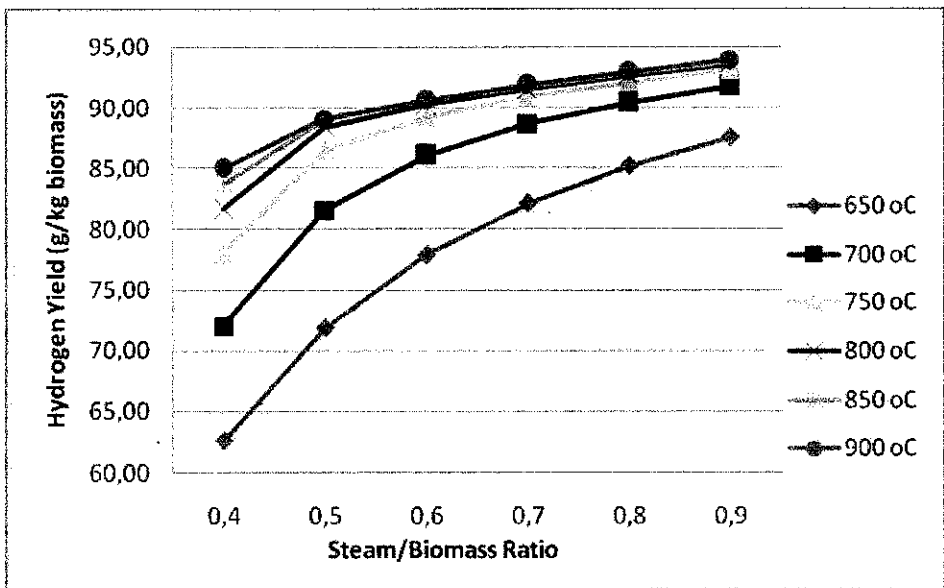


Figure 4.8: Effect of Steam/Biomass Ratio on Hydrogen Yield at Different Gasification Temperature for Empty Fruit Bunches

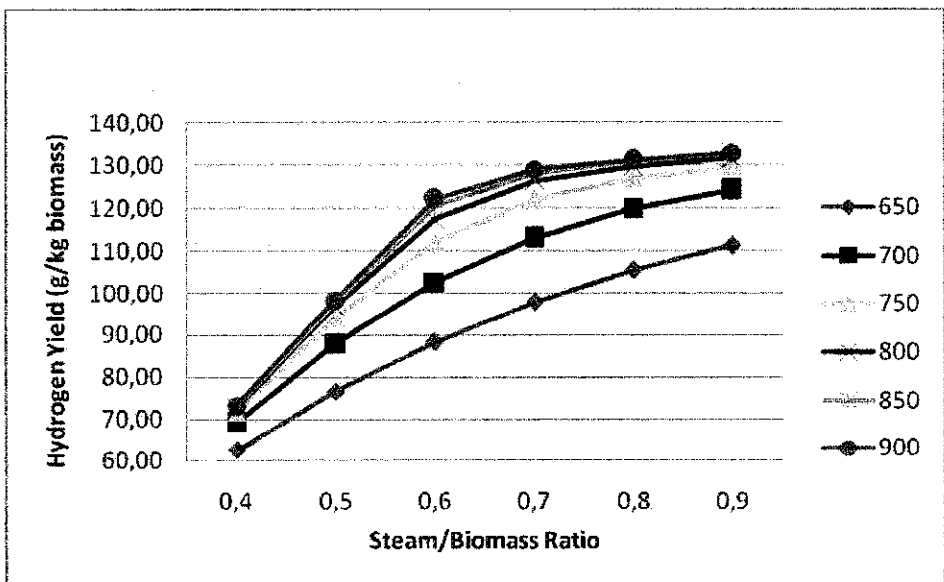


Figure 4.9: Effect of Steam/Biomass Ratio on Hydrogen Yield at Different Gasification Temperature for Rice Husk

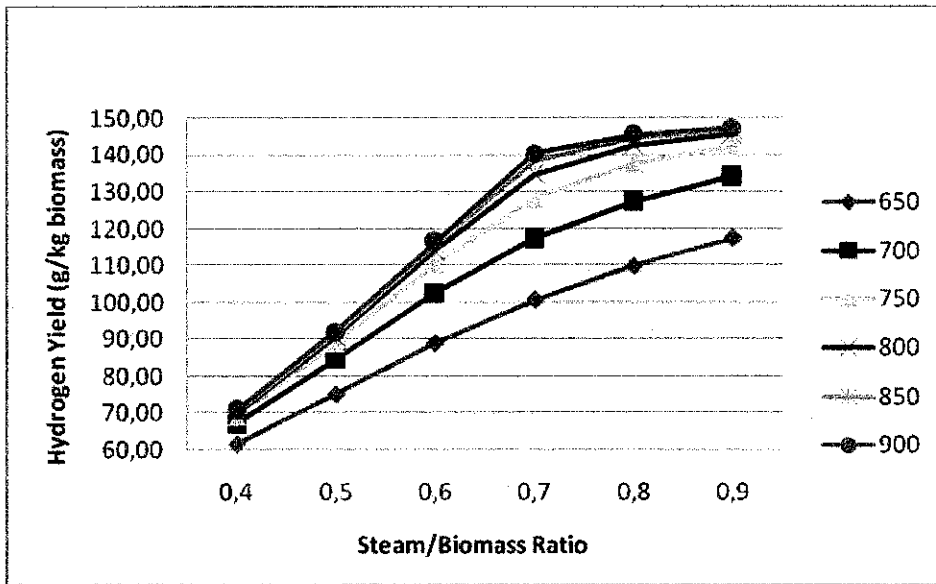


Figure 4.10: Effect of Steam/Biomass Ratio on Hydrogen Yield at Different Gasification Temperature for Rubber Wood

The effect of the steam/biomass ratio on hydrogen yield efficiency is shown in Figure 4.8, Figure 4.9 and Figure 4.10 respectively. It was observed that hydrogen yield reached maximum for steam/biomass ratio of 0.7 to 0.9 which is almost similar with the result that was obtained by Shen et.al (2007) which is 0.7. The best gasifier temperature is at 800 °C to 900°C. Hydrogen yield could reach maximum as the steam/biomass ratio increased.

From the analysis of the result of varying steam/biomass ratio, it can be agreed that the introduction of steam in biomass steam gasification benefit in increasing the gas and hydrogen yields. However, excessive steam will lower the reaction temperature and cause hydrogen composition to decrease as Figure 4.5, Figure 4.6 and Figure 4.7 illustrates. In addition, a high content of steam in gas could be a waste of energy (Wei et al., 2006).

Biomass feedstocks contain a high proportion of volatile material. A relatively large fraction of most biomass feedstocks can be devolatilized rapidly at low to moderate temperatures and the organic volatiles can be rapidly converted to gaseous

products. Temperature did affect the process which biomass produces more tar and unburned hydrocarbon in lower temperatures and decreases hydrogen production. Therefore, the temperature in Reactor 1 (R-1) was crucial for hydrogen production from biomass gasification. Higher temperatures favor the reactants in exothermic reactions and favor the products in endothermic reactions (Shen et al., 2008). The use of steam in biomass gasification could increase hydrogen yields by reaction of residual char, which formed via the steam-carbon reaction. Steam gasification also makes it possible to use green biomass feedstock without drying. The use of oxygen to meet any heat requirements would be expected to increase the yields of carbon dioxides. For effect of pressure, the biomass feedstock is in solid, thus pressurizing becomes more complicated at higher pressures (Higman & van der Burgt, 2003).

4.3 Analysis of Data

In order to validate the simulation results, experimental data from gasification of rice husk was used.

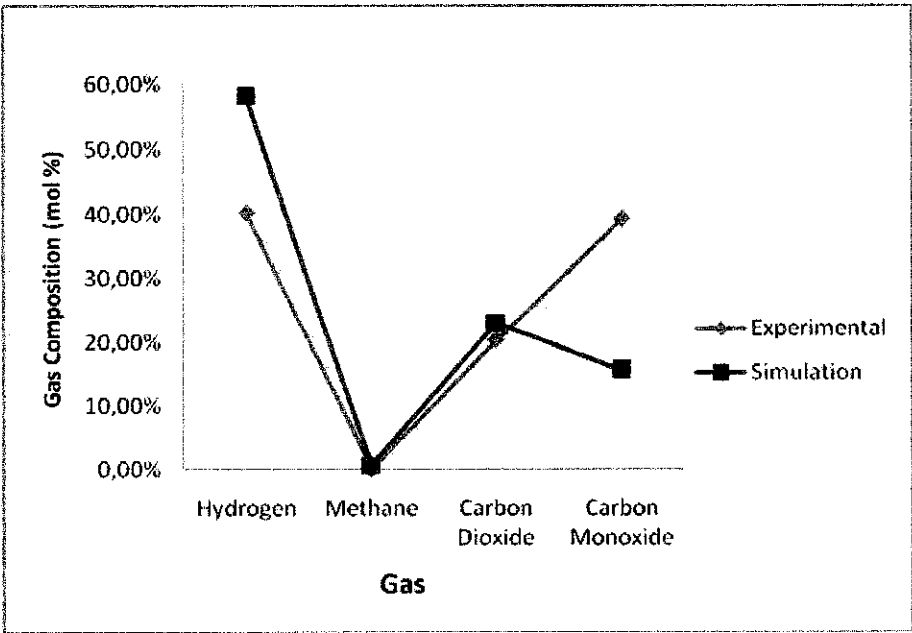


Figure 4.11: Comparison Experimental and Simulation Result for Gas Composition of Rice Husk Gasification

Figure 4.11 show the simulation results compared with experimental data for product gas composition. The feedstock that selected for comparison of product gas composition is rice husk, because rice husk obtained the highest gas yield in this simulation.

Table 4.1: Analysis of Data

	Hydrogen	Methane	Carbon Dioxide	Carbon Monoxide
Mean Error	0.31	0.86	0.12	0.60

The mean error quite big for all gas composition because simulation cannot predict the real trends because effect of varying temperature resulting from the entering steam is ignored (Shen et.al., 2007). From observation of Table 4.1, maybe ICON simulation is not suitable for gas-solid reaction.

4.4 Economic Potential

The economic potential calculation is based on rice husk because rice husk produce the highest hydrogen yield in the simulation. The feasibility of the project is determined using the economic potential of the first level calculation. The raw materials of the gasification process in this project that need to calculated are steam and oxygen because considering the biomass that we can get for free while the product of the process is hydrogen. The current prices of steam, oxygen and hydrogen are as in Table 4.2:-

Table 4.2: Products and Raw Materials Data

	Products		Raw Materials	
	Price	Flow rate	Price	Flow rate
Steam	-	-	RM 15.46/MT	52.5 kg/hr
Oxygen	-	-	RM 92.40/MT	10.5 kg/hr
Hydrogen	RM 8800/MT	9.67 kg/hr	-	-

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

$$\begin{aligned}
 &= \left[\frac{RM8800}{MT} \times \frac{9.67kg}{hr} \times \frac{1MT}{1000kg} \right] \\
 &\quad - \left[\left(\frac{RM15.46}{MT} \times \frac{45kg}{hr} \times \frac{1MT}{1000kg} \right) + \left(\frac{RM92.40}{MT} \times \frac{10.5kg}{hr} \times \frac{1MT}{1000kg} \right) \right] \\
 &= RM 85.09 - RM 1.66 \\
 &= \mathbf{RM 83.43/hr > > 1}
 \end{aligned}$$

Economic Potential 1 (EP1) for this project is more than 1, thus it means that it will bring profit. The hydrogen production is economic feasible.

CHAPTER 5

CONCLUSION AND RECOMMENDATION

5.1 Conclusion

Overall, almost all the objectives of the project were achieved, to simulate the gasification technology using multi feed stock basis and also has to find ways to obtain rich hydrogen gas. Multi feedstock such as empty fruit bunches, rice husk and rubber wood that can be simulated using same simulation. The simulation shows the temperature increases the production of hydrogen and enhances carbon conversion efficiency while carbon monoxide and methane show decreasing trends. From this project, it is suggested the best reactor temperature is 900°C and steam/biomass ratio between 0.7-0.9 to obtain maximum hydrogen yield.

5.2 Suggestion Future Work for Expansion and Continuation

It was necessary to modify the ICON simulation software to support solid reaction. The simulation shows that the biomasses were detected in oils compound and not in solid compound. Thus, the results were not accurate due to drawback in using ICON simulation software. Detailed experimental data about the influence of operating conditions along with the kinetics studies is needed to obtain a thorough evaluation.

REFERENCES

- Basu, P. (2006). *Combustion and Gasification in Fluidized Beds*. United States of America: CRC Press, Taylor & Francis Group.
- Belonio, A.T. (2005). *Rice Husk Gas Stove Handbook*. Appropriate Technology Center. Department of Agricultural Engineering and Environmental Management, College of Agriculture, Central Philippine University, Iloilo City, Philippines.
- Bhattacharya, S. C. (1997). State of the art of biomass gasification. *Proc. Of the International Symposium on Advances in Alternative and Renewable Energy* , 50-57.
- Chauvel, A. (1989). *Petrochemical Processes*. Paris: Editions Technip.
- Deraman, M. (1993). Carbon pellets prepared from fibers of oil palm empty fruit bunches: 1. A quantitative X-ray diffraction analysis. *PORIM Bull. Palm Oil Res. Inst. Malaysia* , 26.
- Gasification Technologies Council*. (2008). Retrieved August 20, 2008, from What is Gasification?: http://www.gasification.org/what_is_gasification/overview.aspx
- Hanping C., Bin L., Haiping Y., Guolai Y., and Shihong Z. (2008). *Experimental Investigation of Biomass Gasification in a Fluidized Bed Reactor*. Energy & Fuels. American Chemical Society. New York
- Hashim, H., & Chong, L. (2007). ICON-PI Online Model for MTBE Propane Refrigerant Flaring Monitoring. *OSIsoft Asia Technology Conference*.
- Higman, C., & van der Burgt, M. (2003). *Gasification*. United States of America: Elsevier.
- Hussain, A., Ani, F. N., Darus, A. N., Mokhtar, H., Azam, S., & Mustafa, A. (2006). Thermochemical Behaviour of Empty Fruit Bunches and Oil Palm Shell Waste in a Circulating Fluidized Bed Combustor (CFBC). *Journal of Oil Palm Research* , 210-218.
- Hutchison, F. (2006, July 6). *Facts about gasification*. Retrieved August 15, 2008, from clean-energy.us:: <http://www.clean-energy.us/facts/gasification.htm>

HYSYS Integrated Engineering Environment (1997). Retrieved September 2, 2008 from Hyprotech Ltd. :: <http://www.ccr.jussieu.fr/ccr/Documentation/Calcul/matlab5v11/docs/00058/058f3.htm>

Laihong Shen, Yang Gao, Jun Xiao. (2008). Simulation of Hydrogen Production From Biomass Gasification in interconnected Fluidized Beds. *Biomass And Bioenergy* , 120-127.

lv P., Chang J, Xiong Z., Huang H., Wu C., Chen Y., and Zhu J. (2002). *Biomass Air-Steam Gasification in a Fluidized Bed to Produce Hydrogen-Rich Gas*. Energy & Fuels. American Chemical Society. New York

Maeland. A. (2006). *Hydrogen Production. Based on Russian Hydropower.* :: <http://www.rosnor.com>

Nath K. & Das D. (2003). Hydrogen from Biomass. *Current Science*, vol 85, no 3 , 265-271.

Nemtsov, D., & Zabaniotou, A. (2008). Mathematical modelling and simulation approaches of agricultural residues air gasification in a bubbling fluidized bed reactor. *Chemical Engineering Journal* .

Pröll T., Hofbauer H. (2008). H₂ rich syngas by selective CO₂ removal from biomass gasification in a dual fluidized bed system — *Process modeling approach*, *Fuel Process. Technol.* Doi:10.1016/j.fuproc.2008.05.020

Rifkin, J. (2006). *The Hydrogen Economy*. Retrieved August 17, 2008, from Renewable Energy World.Com:: Rifkin 2006, <http://www.renewableenergyworld.com/rea/news/reinsider/story?id=41130>

Scahill, J. (2003). Biomass to Energy: Present Commercial Strategies and Future Option. *Bioenergy and Wood Products Conference*.

Simulation Application in Thermodynamic (2006). Introduction. *ICON Process Simulation Software Training Course 2006*.

Srinivasakannan C. and Zailani A.B (2003). *Production of Activated Carbon From Rubber Wood Sawdust*. Biomass and Bioenergy 27 , 89 – 96

Wei L., Xu S., Liu J., Lu C., Liu S., and Liu C. (2006). *A Novel Process of Biomass gasification for Hydrogen-Rich Gas with Solid Heat Carrier: Preliminary Experimental Results*. Energy & Fuels. American Chemical Society. New York

APPENDICES

APPENDIX I CALCULATION

FEEDSTOCKS

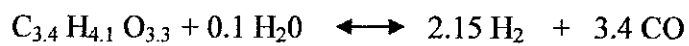
Empty Fruit Bunches

Chemical Formula = $C_{3.4} H_{4.1} O_{3.3}$

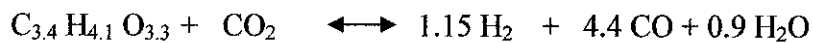
Molecular Weight = $3.4(12) + 4.1(1) + 3.3(16) = 97.7$

Density = 450 kg/m^3

Reaction 1 – Steam Gasification



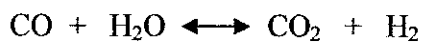
Reaction 2 – Boudouard



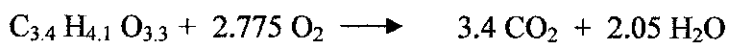
Reaction 3 – Methanation



Reaction 4 – Water Gas Shift



Reaction 5 – Combustion



Reaction 6 – Steam Reforming



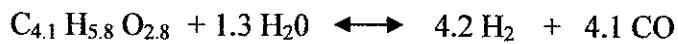
Rice Husk

Chemical Formula = $C_{4.1} H_{5.8} O_{2.8}$

Molecular Weight = $4.1(12) + 5.8(1) + 2.8(16) = 99.8$

Density = 1063 kg/m^3

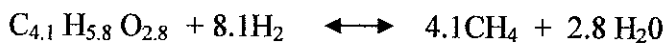
Reaction 1 – Steam Gasification



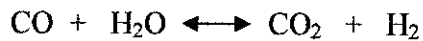
Reaction 2 – Boudouard



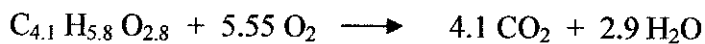
Reaction 3 – Methanation



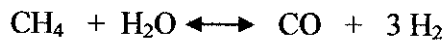
Reaction 4 – Water Gas Shift



Reaction 5 – Combustion



Reaction 6 – Steam Reforming



Rubber Wood

Chemical Formula = $C_4 H_6 O_{2.4}$

Molecular Weight = $4(12) + 6(1) + 2.4(16) = 92.4$

Density = 626 kg/m^3 (Rubberboard of India, 2008)

Reaction 1 – Steam Gasification



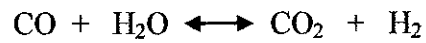
Reaction 2 – Boudouard



Reaction 3 – Methanation



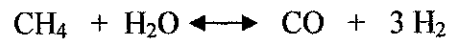
Reaction 4 – Water Gas Shift



Reaction 5 – Combustion



Reaction 6 – Steam Reforming



REACTION CONSTANT (need to include in the reactor simulation)

Steam Gasification Reaction

T (°C)	T(K)	K_exp
600	873	0,10520734
650	923	0,11885651
700	973	0,13260357
750	1023	0,14636629
800	1073	0,16007743
850	1123	0,17368255
900	1173	0,18713807
950	1223	0,20040955
1000	1273	0,21347015
1050	1323	0,22629943

$$K_{exp} = \exp \left[\frac{-G}{(R T)} \right]$$
$$= \exp[-16344/(8,314 \cdot T(K))]$$

Where

$$\Delta \tilde{G}_{0,i}$$

Steam Gasification	16344
Boudouard	20294
Methanation	-11005

Boudouard Reaction

T (°C)	T(K)	K_exp
600	873	0,061051343166
650	923	0,071035517208
700	973	0,081375805968
750	1023	0,091991092560
800	1073	0,102809556420
850	1123	0,113768310526
900	1173	0,124812793848
950	1223	0,135896042922
1000	1273	0,146977922725
1050	1323	0,158024366800

Methanation Reaction

T (°C)	T(K)	K_exp
600	873	4,555031453165
650	923	4,195851647717
700	973	3,897758967112
750	1023	3,647022073607
800	1073	3,433626131651
850	1123	3,250119686810
900	1173	3,090859489579
950	1223	2,951503588203
1000	1273	2,828663485473
1050	1323	2,719660666483

H₂ yield efficiency

$$\text{H}_2 \text{ yield efficiency} = \frac{\text{H}_2 \text{ yield in the gasifier (g)}}{\text{Biomass fed into the system (kg)}}$$

APPENDIX II STREAMS SIMULATION IN ICON

Biomass

EmptyFruitBunches* Properties

Identifier

Basic Properties

T-dep Properties

Other Properties

Name

EmptyFruitBunches*

Formula

C5.82163E+000H1.56433E+001

CASN

-1238917730[OIL.EmptyFruitBunches*]

ChemicalFamily

Oils

UNIFACStruct...

Notes

CreationInfo:

Name = EmptyFruitBunches*

MolecularWeight = 97.7

LiquidDensity@298 = 450

OK

Print

Edit...

EmptyFruitBunches* Properties

Identifier

Basic Properties

T-dep Properties

Other Properties

MolecularWeight

97.70

NormalBoilingPoint

C

300.2935

LiquidDensity@298

kg/m3

450.000

CriticalPressure

kPa

78.951

CriticalVolume

m3/kmol

16.194

CriticalTemperature

C

339.3649

CriticalCompressibility

0.2510

AcentricFactor

0.4466

CreationInfo:

Name = EmptyFruitBunches*

MolecularWeight = 97.7

LiquidDensity@298 = 450

OK

Print

Edit...

/Biomass (Stream_Material)

Name:

Biomass

Description:

Solved

Spec From

...

☐ Detail View

☐ Exclude From Summary

Summary

Equilibrium Results

Line Sizing

Material

Connected to [In|Out]

/M-1.In1

VapFrac

0.00

T [C]

30.00

P [kPa]

100.0

MoleFlow [kgmole/h]

0.77

MassFlow [kg/h]

75.00

VolumeFlow [m3/hr]

0.209

StdLiqVolumeFlow [m3/hr]

0.167

StdGasVolumeFlow [SCMD]

4.3646E+2

± Properties

± Mole

[Fraction]

[kgmole/h]

± Mass

[Fraction]

[kg/h]

± StdLiqVolume

[Fraction]

[m3/hr]

Print

Create Port

Delete Port

☐ Ignored

Oxygen

oxygen (Stream_Material)

Name: oxygenDescription:

Solved

Spec From

...

Detail View

Exclude From Summary

SummaryEquilibrium ResultsLine Sizing

Material

Connected to [In Out]	/M-1.Jn2
VapFrac	1.00
T [C]	900.00
P [kPa]	100.0
MoleFlow [kgmole/h]	0.45
MassFlow [kg/h]	14.25
VolumeFlow [m3/hr]	43.446
StdLiqVolumeFlow [m3/hr]	0.032
StdGasVolumeFlow [SCMD]	2.532E+2

Properties

+

 Mole

[Fraction]

[kgmole/h]

+

 Mass

[Fraction]

[kg/h]

+

 StdLiqVolume

[Fraction]

[m3/hr]

Print

Create Port

Delete Port

Ignored

Steam

/Steam (Stream_Material)

Name: SteamDescription:

Solved

Spec From

Detail View

Exclude From Summary

SummaryEquilibrium ResultsLine Sizing

Material

Connected to [In|Out]

/M-1.In0

VapFrac

1.00

T [C]

145.00

P [kPa]

100.0

MoleFlow [kgmole/h]

1.67

MassFlow [kg/h]

30.00

VolumeFlow [m3/hr]

57.518

StdLiqVolumeFlow [m3/hr]

0.030

StdGasVolumeFlow [SCMD]

9.4681E+2

Properties:

+

Mole

[Fraction]

[kgmole/h]

+

Mass

[Fraction]

[kg/h]

+

StdLiqVolume

[Fraction]

[m3/hr]

Print

Create Port

Delete Port

Ignored

Reactor 1 (R-1)

/R-1 (EqmReactor)

Name: **R-1** Description:

Type: ☒ Equilibrium Reactor ☐ Gibbs Reactor

Summary | **Reactions** | Reaction Constants | Settings | Schematic

Main Data

Name	Value
Energy Out	
OutQ [W]	40000.00
Signal	
Delta P [Kpa]	0.00

Material

PortName	In	Out
Is Recycle Port	☐	☐
Connected Stream/Unit Op	/S1.Out	/S2.In
VapFrac	0.1588	1.00
T [°C]	43.0051	1000.00
P [kPa]	100.0	100.0
MoleFlow [kmole/h]	2.88	2.89
MassFlow [kg/h]	119.25	119.25
VolumeFlow [m³/hr]	12.308	305.257
StdLiqVolumeFlow [m³/hr]	0.229	0.229
StdGasVolumeFlow [SCMD]	1.6365E+3	1.6444E+3
* Properties (All+R)		
* Fraction [Fraction]		
HYDROGEN	0.0000	0.0016
METHANE	0.0000	0.00292
CARBON DIOXIDE	0.0000	0.00522
CARBON MONOXIDE	0.0000	0.0000
WATER	0.57857	0.57324
OXYGEN	0.15472	0.15398
EmptyFruitBunches*	0.26671	0.26303
* MassFraction [Fraction]		
* StdVolFraction [Fraction]		
* MoleFlow [kmole/h]		
* MassFlow [kg/h]		
* StdLiqVolumeFlow [m³/hr]		

Print Ignored

/R-1 (EqmReactor)

Name: **R-1** Description:

Type: ☒ Equilibrium Reactor ☐ Gibbs Reactor

Summary | **Reactions** | Reaction Constants | Settings | Schematic

Rxn Name	Rxn0	Rxn1	Rxn2
steam_gasification	OXYGEN	CARBON DIOXIDE	HYDROGEN
Base Comp			
HYDROGEN	2.15	1.15	-8.05
METHANE			3.4
CARBON DIOXIDE		-1	
CARBON MONOXIDE	3.4	4.4	
WATER	-0.1	0.9	3.3
OXYGEN			
EmptyFruitBunches*	-1	-1	-1
Balance	0.0670	0.0670	0.0670
H Rxn(25 °C)[kJ/mol]		-1.27E+05	-1.08E+05

methanation: 3.4*METHANE+3.3*WATER-8.05*HYDROGEN-1.0

Print Ignored

R-1 (**E.qnReactor**)

Name: **R-1** Description:

Type: ☒ Equilibrium Reactor ☐ Gibbs Reactor

Summary | Reactions | Reaction Constants | Settings | Schematic

Equilibrium Constant: **K-T Table**

Calculation Basis: **Vapor Partial Pressure** Units: **kPa**

Equilibrium Constant - Temperature

Rm0				Rm1	
Reaction Constant is 2.67067E-06				Reaction Constant is ...	
T (C)	K _{exp}	K _{cal}	Error (%)	T (C)	K _{exp}
700.00	5.00E-08	5.04E-08	0.7847	700.00	8.75E-10
750.00	1.20E-07	1.17E-07	-2.57	750.00	2.42E-08
800.00	2.40E-07	2.46E-07	2.50	800.00	6.11E-08
850.00	4.80E-07	4.80E-07	0.0366	850.00	1.42E-08
900.00	8.90E-07	8.85E-07	-0.5686	900.00	3.06E-08
950.00	1.57E-06	1.56E-06	-0.5126	950.00	6.22E-08
1000.00	2.66E-06	2.67E-06	0.4010	1000.00	1.19E-07

Regression Equation: $K_{cal} = \text{Exp}(A + B/T + C \log(T) + I)$ Plot Edit...

Print