CERTIFICATION OF APPROVAL

Simulation of Petcoke Gasification in Fluidized Bed Gasifier

by

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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.

ZEELAWATI BINTI RAZAK

ABSTRACT

Gasification technology has been viewed as an alternative way to produce energy by the industries. The process transforms low value feedstock and turns it into valuable gaseous products. Petroleum coke or petcoke is a byproduct from oil refineries with high carbon content. This gives petcoke more preferred feedstock to produce power. The study will be focusing on developing a simulation on the petcoke gasification in a fluidized bed gasifier by using the ASPEN HYSYS process simulator. The effect of oxygen to coke ratio and steam to coke ratio and the temperature with respect to the gasification performance will also be examined in the model simulation.

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CHAPTER 1

1. INTRODUCTION

1.1. Background of Study

Natural gas consumption represents almost 46% of this primary energy consumption. The main applications of natural gas are chemistry, power production, and largest is on the production of heat for both households and industry. Both natural gas and coal remains as the world's most important sources of supply in 2030, with a 64 % share of total generation as shown in figure 1 [1].

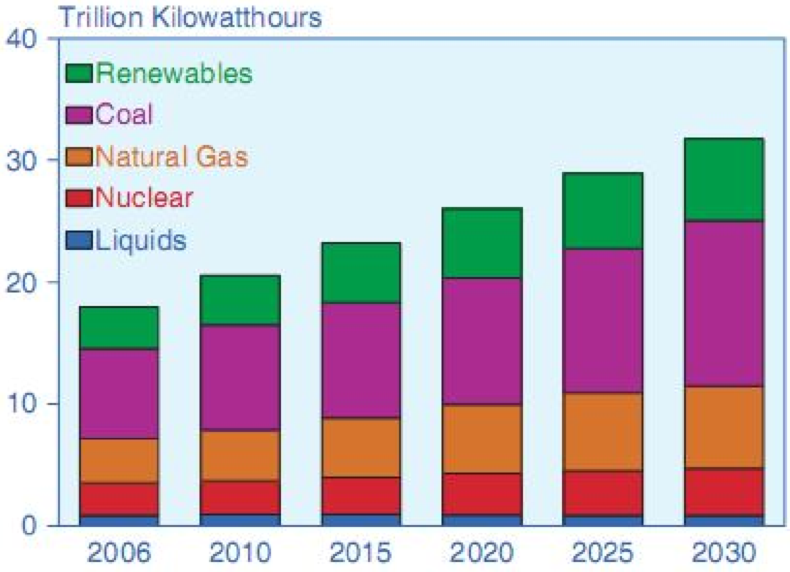


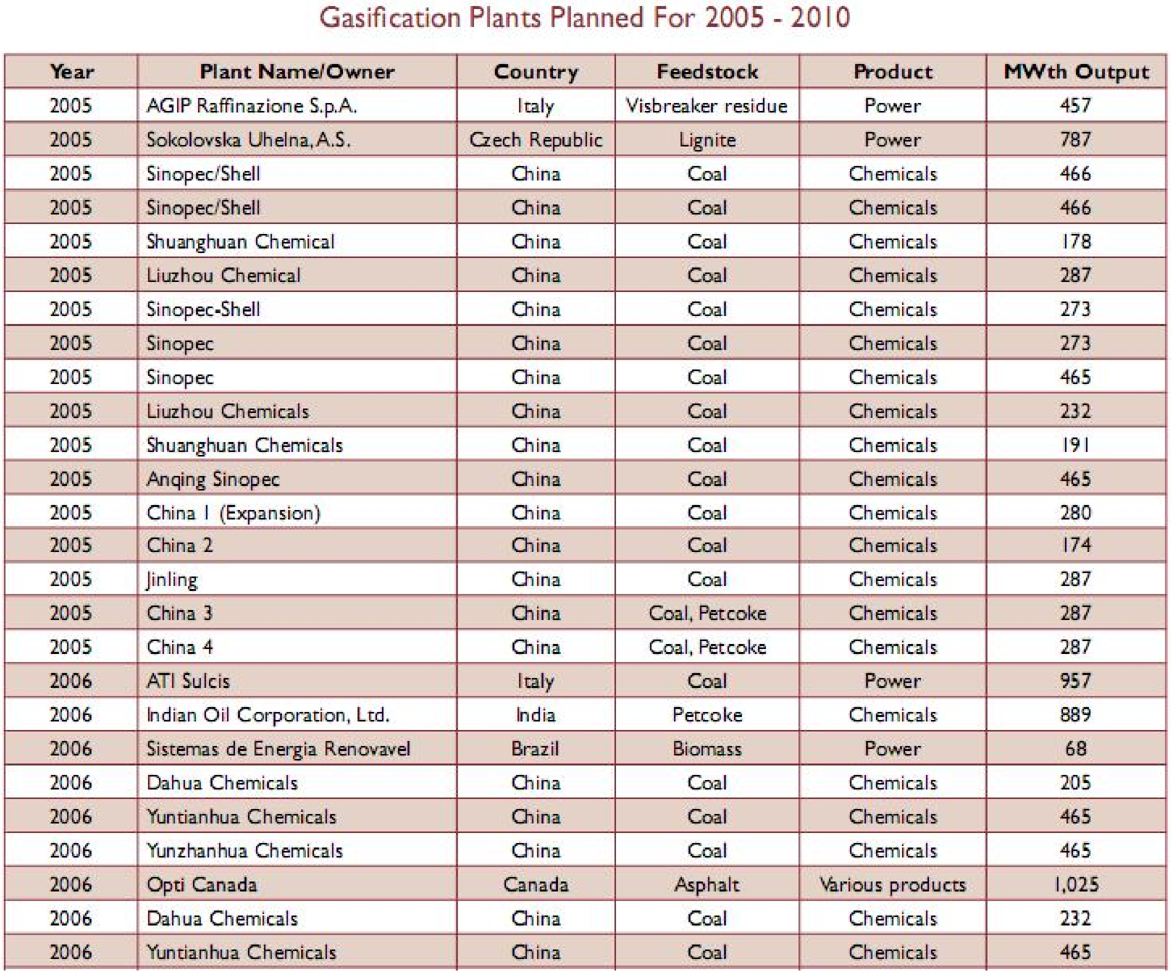
Figure 1.1: World Electricity Generation by Fuel, 2006-2030

Increasing in the natural gas price has make industries to look for other alternative sources to produce energy. Gasification had been viewed as the solution to overcome this problem. The gasification process transforms cheap and low value feedstock into valuable gaseous products. The technology also gained greater attention due to its ability to produce cleaner energy.

World gasification capacity is projected to grow by more than 70% by 2015. More than 80% of the growth will occur in Asia, with China expected to achieve the most rapid expansion in gasification worldwide.

Despite the high construction costs and uncertainty about U.S. government policies, incentives, and regulations, gasification is expected to grow in the United States due to high and rising in oil and natural gas prices, more stringent environmental regulations, and a growing consensus that CO_2 management will be required for electric power generation and manufacturing plants [2].

Table 1.1: Gasification Planned for 2005 – 2010



Gasification Plants Planned For 2005 - 2010

Year	Plant Name/Owner	Country	Feedstock	Product	MWth Output
2005	AGIP Raffinazione S.p.A.	Italy	Visbreaker residue	Power	457
2005	Sokolovska Uhelna, A.S.	Czech Republic	Lignite	Power	787
2005	Sinopec/Shell	China	Coal	Chemicals	466
2005	Sinopec/Shell	China	Coal	Chemicals	466
2005	Shuanghuan Chemical	China	Coal	Chemicals	178
2005	Liuzhou Chemical	China	Coal	Chemicals	287
2005	Sinopec-Shell	China	Coal	Chemicals	273
2005	Sinopec	China	Coal	Chemicals	273
2005	Sinopec	China	Coal	Chemicals	465
2005	Liuzhou Chemicals	China	Coal	Chemicals	232
2005	Shuanghuan Chemicals	China	Coal	Chemicals	191
2005	Anqing Sinopec	China	Coal	Chemicals	465
2005	China 1 (Expansion)	China	Coal	Chemicals	280
2005	China 2	China	Coal	Chemicals	174
2005	Jinling	China	Coal	Chemicals	287
2005	China 3	China	Coal, Petcoke	Chemicals	287
2005	China 4	China	Coal, Petcoke	Chemicals	287
2006	ATI Sulcis	Italy	Coal	Power	957
2006	Indian Oil Corporation, Ltd.	India	Petcoke	Chemicals	889
2006	Sistemas de Energia Renovavel	Brazil	Biomass	Power	68
2006	Dahua Chemicals	China	Coal	Chemicals	205
2006	Yuntianhua Chemicals	China	Coal	Chemicals	465
2006	Yunzhanhua Chemicals	China	Coal	Chemicals	465
2006	Opti Canada	Canada	Asphalt	Various products	1,025
2006	Dahua Chemicals	China	Coal	Chemicals	232
2006	Yuntianhua Chemicals	China	Coal	Chemicals	465

2006	Yunzhanhua Chemicals	China	Coal	Chemicals	465
2006	Shenhua	China	Coal	Hydrogen	861
2006	China 5	China	Coal	Chemicals	284
2007	Yongcheng Chemicals	China	Coal	Chemicals	424
2008	Global Energy, Inc.	United States	Coal, MSW	Power	1,006
2008	Vanguard Synfuels	United States	Petcoke	Various products	0
2008	Lotos Reffinery Gdansk	Poland	Asphalt	Various products	620
2009	Excelsior Energy	United States	Coal	Power	0
2009	Lake Charles Cogeneration LLC	United States	Petcoke	Various products	0
2009	Rentech Development	United States	Coal	FT liquids	59
2009	Qatar Petroleum	Qatar	Natural Gas	FT liquids	10,936
2010	Steelhead Energy	United States	Coal	Power	0

Coal gasification results in either to produce syngas or to generate electricity in an IGCC plant [10]. The technology has existed since the last decades. High ash content presence in coal makes petcoke and biomass as more preferable gasification feedstock. Petcoke from oil refineries are low in cost, higher energy content, and greater availability. However, petcoke contains higher sulfur compared to coal and this can lead to corrosion and environmental emission problems [3].

Gasification takes place in a fluidized bed gasifier cause perfect mixing between gas and solid, thus improve the heat and mass transfer characteristics [4]. Several works on the simulation of biomass gasification in fluidized bed reactor has been investigated but limited for petcoke gasification [4-5].

The purpose of this study is to develop simulation of petcoke gasification in a fluidized bed gasifier. By using the process simulator ASPEN HYSIS, the gasification will be performed in a fluidized bed reactor and the operating parameters will be controlled to produce the desired syngas concentration.

In the second part, review on the gasification process, types of gasifier, gasification reactions and petcoke properties had been discussed in details. The third part is on the methodology for the final year project research. Basically the first phase in the research methodology is doing literature review on the background of the process and the second phase is which the simulation process will take place. And the last part will be on the updated work progress so far regarding the project.

1.2. Problem Statement

Energy drives human activities and development. Depletion in oil and gas resources resulted in using alternative source to produce energy. By the year 2020, Middle East will be the only major reservoir of abundant crude oil as shown in Figure 1 [6].

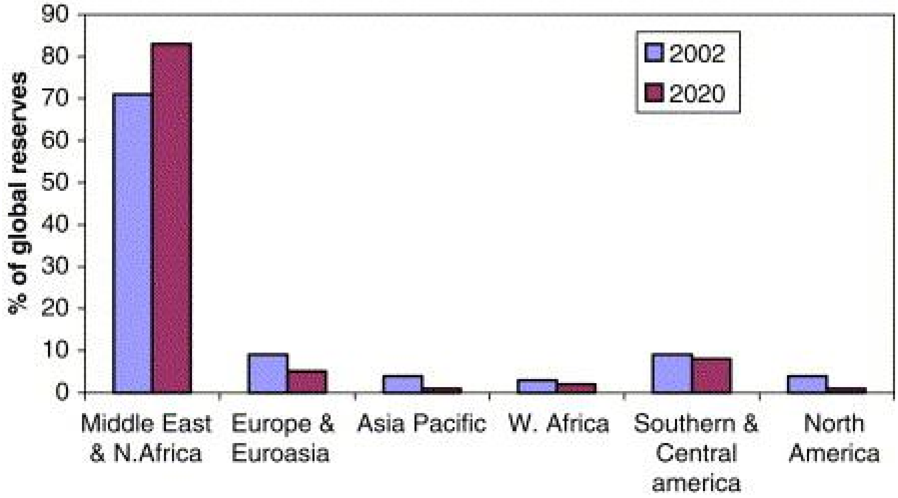


Figure 1.2: BP statistical review of world energy: world reserves for 2002 and 2020

1.2.1. Significant of the Project

Continuation used of fossil fuels is set to face multiple challenges such as the depletion of fossil fuel reserves, global warming and other environmental issues. Besides, depleting in these resources had caused high in oil and gas price. This can be solved by using an alternative source to replace the fossil fuel. Gasification transforms the low value feedstock into more valuable gaseous products.

Historically, refineries have utilized natural gas to produce hydrogen. Now, with the increasing price of natural gas, refineries are looking to alternative sources to produce the needed hydrogen.

Petcoke from the oil refineries can be gasify to produce syngas (H_2 and CO) which can be further processed to produce chemicals, fertilizers, liquid fuels, hydrogen, and electricity. In addition, this will meet the refineries hydrogen and energy demand.

1.3. Objective and Scope of Study

1.3.1. Objectives

1. To study the different types of gasifiers and select the suitable gasifier for petcoke gasification
2. To develop process model for simulation of petcoke gasification in a fluidized bed gasifier
3. To study the effect of variation in model parameters (temperature, oxygen to coke ratio, and steam to coke ratio) towards syngas composition

1.3.2. Scope of Study

The study consists of two phases. The first phase focuses on the background of the gasification process. Here is where many works on the literature review will be done. Some articles and journals related to the study will be discussed. Thus, further understanding about the process can be gained.

The second phase will be on developing the simulation of the process. The simulation will be conducted using the ASPEN HYSIS process simulator. The data resulted from the simulation will be further validated using the data taken from experimental works.

1.4. The Relevancy of the Project

Refineries consume natural gas to generate power for the plant requirements. However, the natural gas price kept increasing [3].

Petcoke act as a substitute for the natural gas to produce energy through the gasification process. This is more preferable compared to coal due to its high energy content. Besides, other byproducts obtained from the refining process such as petroleum coke, asphalts, tars, and some oily wastes can be further gasified to generate both the required hydrogen, and the power and steam needed to run the refinery [7].

Gasification is a link technology to a hydrogen economy. It can become a competitive route to produce large quantities of hydrogen that will later needed for fuel cells and cleaner fuel. This contrast to the other technologies that must first separated the hydrogen from water using electricity and more expensive of natural gas. The technology converts low value of residuals into high value products such as chemicals and fertilizers, substitute natural gas, transportation fuels, electric power, steam, and hydrogen. [8]

1.5. Feasibility of the Project within the Scope and Time Frame

Sufficient time was given to conduct this study. First half of the year will be mainly on the background of study of the process and another half year will be on the simulation itself. Better understanding on the study can be achieved before starts to conduct the simulation. Hence, it will be easier in doing the simulation.

CHAPTER 2

2. LITERATURE REVIEW

2.1. Gasification

Gasification is a process that converts carbonaceous materials such as coal, petroleum coke (petcoke), and biomass to synthesis gas (syngas), which can be further processed to produce chemicals, fertilizers, liquid fuels, hydrogen, and electricity [9].

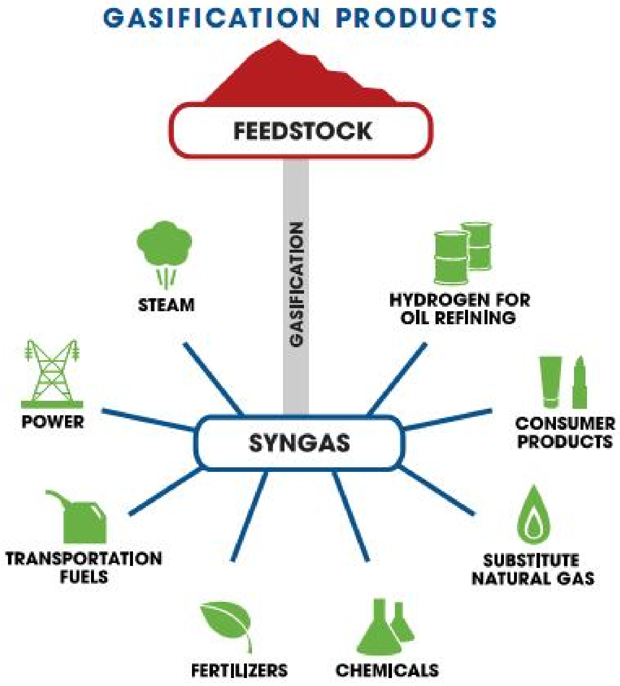


Figure 2.1: Examples on the gasification products

Gasification can be carried out in three types of reactors which are the moving bed reactor, fluidized bed reactor, and entrained flow reactor.

2.2. Types of Gasifier

Different gasifier will perform differently depending on its feed types and size. Hence, the right chosen reactor will ensure the optimization of the efficiency [10].

2.2.1. Moving Bed Processes

Moving bed gasifier is a countercurrent flow reactor. The feed enters on the top of the reactor and the gasification agent enters from the bottom. The feed undergoes gasification reactions as it move downwards and the remaining ash will drop at the bottom of the reactor. As a result of the countercurrent flow, heat from the gasification reactions will preheat the feed enters at the top of the reactor [11]. The generic diagram on the moving bed gasifier is being shown in figure 2.

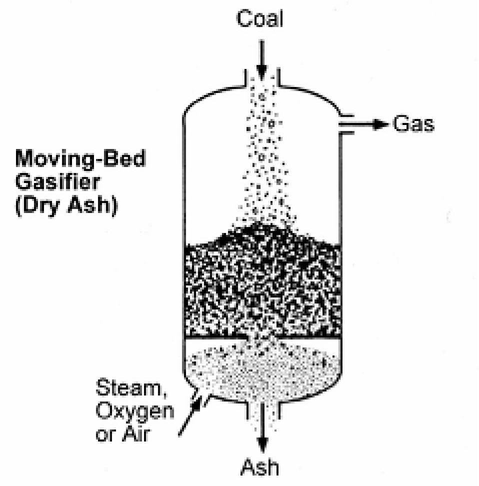


Figure 2.2: Diagram of a generic moving bed gasifier

In order to run a fixed-bed dry bed gasifier, the temperature in the gasifier must be kept below that of ash fusion (1000°C – 1300°C). Fixed-bed gasifiers have the advantages of high thermal efficiency and low temperatures (425°C-650°C) for the outlet gas. But they also are plagued by low throughput and produce significant amounts of tar and methane that require separation.

2.2.2. Fluidized Bed Processes

Fluidized bed gasifier is also known as a back-mixed or well-stirred reactor. New feed particles will mix with the older, partially gasified, and fully gasified particles inside the reactor. Hence, the mixing will develop uniforms temperature throughout the bed. The flow of the gasifying agents and recycled syngas should be sufficient enough to lift the particles inside the bed [11].

A fluidized bed gasifier operates at temperature lowers than its ash softening point, typically in the range of 950-1100°C for coal and 800-950°C for biomass. This is to prevent agglomeration problems inside the bed [book].

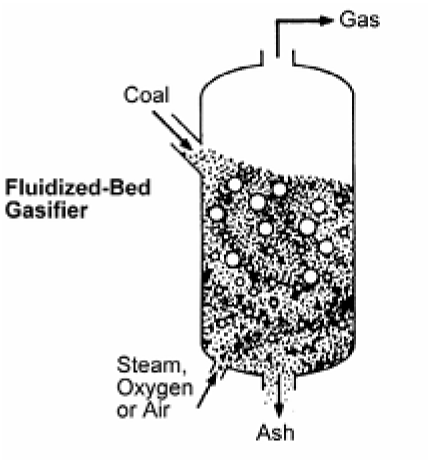


Figure 2.3: Diagram of a generic fluidized bed gasifier

2.2.3. Entrained Flow Processes

An entrained flow gasifier is preferable for large scale systems. High temperature inside the reactor allows the production of tar free gas and with nearly complete carbon conversion [10].

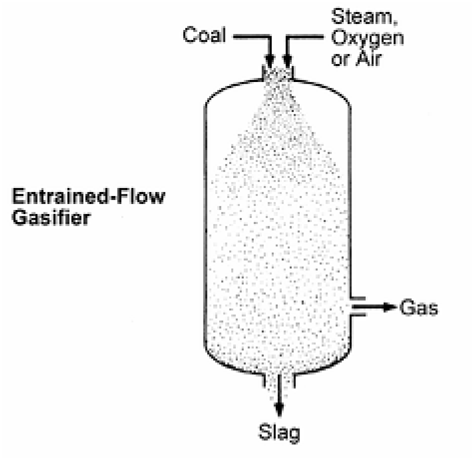


Figure 2.4: Diagram of a generic entrained flow gasifier

Finely pulverized fuel, on the scale of 100-600 microns, is gasified within seconds at high temperatures of around 1500°C – 1900°C. The feed is entrained with oxygen and steam in a co-current flow, which requires an air separation unit, in turn increasing costs and energy use. The gasification process quick reaction time allows for a very high throughput, less problem with caking fuels, and highly efficient of carbon conversion [12].

Table 2.1: Comparison of Fixed Bed and Fluidized Bed gasifiers

Reactor type	Fixed bed		Fluidized bed	
Criteria	Updraft	Downdraft	Bubbling bed	Circulating bed
Technology Designed hours of operation Technical availability/technical features	(-) There is no plant working continuously at design parameters for more than 5000 h/a (+) Simple and robust construction (-) Internal moving parts with some mechanical complications (-) Bad temperature distribution (-) Hot spots with exothermic reaction (-) Poor heat exchange (-) Possible ash agglomeration and clinker formation on grate (-) Channelling possible (-) Residence time for solids: hours to days. For gas:		(-) There is no plant working continuously at design parameters for more than 5000 h/a (+) Less complex technology. No moving parts (+) Good temperature distribution (+) No hot spots (+) Very good heat exchange (-) Conflicting temperature requirement exists for low-reactivity feedstock with low-softening ash melting-point (-) Operation can be more difficult then fixed bed (+) Good gas solid contact and mixing (+) Residence time for solids: seconds to minutes. For gas:	

	seconds (+) Pressure drop is low	seconds (-) Pressure drop is higher than bubbling bed
Experience	(+) Lots of processes for different applications in operation (+) Simple, reliable and proven for certain fuels (-) Low specific capacity (-) High residence time of solids (+) Gasifier may be banked for long periods (-) Very limited scale-up potential caused by low maximum size	(+) Commercial designs are available (+) Large fuel inventory provides safety, reliability and stability (+) High specific capacity (+) High reaction rates, low residence time of solids (+) Gasifier may be banked for long periods (+) Very good scale-up potential
Start-up/shutdown behaviour Load range	(-) Gasifier capacity is limited by gas flow rates (-) Heat transport limits scale-up (-) Long period to heat-up (+) Good turndown (-) Limited turndown	(-) Capacity is limited by entrainment at high gas velocities (+) Easily started and stopped (-) Turndown range is limited by the gas velocity required to maintain fluidization
Load change	(+) Can operate at partial load (20±110%)	(+) Can operate at partial load (50±120%) (+) 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

Space required	(-) More space required for high throughput because of modular combination of single low power reactors (-) Bad temperature profile in bed	(+) Less space requirement because of great scale-up (-) Control possibilities by immersed heat exchangers in bed
Degree of automation Use of material Requirement of educts	(+) High ash content feedstock possible (-) Only for catalysts that are deactivated very slowly (-) Close size specification required on feedstock (-) Large pellets (8±50 mm) as uniform as possible needed (-) Feedstock fines must be handled separately (agglomeration)	(+) Tolerates wide variations in fuel quality (-) In-bed catalytic processing hardly Possible (+) Variety of particle sizes can be Handled (+) Broad particle-size distribution (ca. 0.02±50 mm) (+) High fines content acceptable
Quality of main products	(-) Excess steam for temperature control leads to thermal losses and requires special condensate treatment (+) Amount of tar and phenols in product gas is low (0) Low exit gas temperature (0) High exit gas temperature	(+) Amount of tar and phenols in product gas is low (+) Gas composition is steady due to uniform conditions in the bed (0) Gas exit temperature similar to bed temperature

Quality of co-products Requirement for subsequent treatment	(+) Low dust content in product gas (-) Extensive gas cleanup needed for engines (-) High dust content in product gas (+) Relatively clean gas is produced	(-) Higher particulates in the product gas than at fixed bed (-) Inevitable loss of carbon in ash due to the non uniform solids composition of the bed (-) High dust content in gas phase
Use of energy Efficiency of conversion rate	(+) High carbon conversion efficiency	(+) High carbon conversion efficiency
Internal load		(-) High energy requirement for fans (for fluidizing air) (-) High energy requirement for fans (for fluidizing air) (+) Moderate gasification temperature can be used
Losses Environmental Gas emissions Waste water	(-) No primary gas cleaning possible (0) Depends on pre-treatment (+) Molten slag possible	(+) Primary gas cleaning possible (0) Depends on pre-treatment (-) Ash not molten

Economic Total investment Total operating cost (Development) Potential	(-) High investment for big plants	

[a] (+), Advantage; (0), neutral; (-), limitation.

Source: R. Warnecke / Biomass and Bioenergy 18 (2000) 489-497

2.3. **Basic Gasification Reactions in Fluidized Bed Gasifier**

Solid carbons presence either in the form of coal, coke, or char will undergoes these chemical reactions during the gasification.

1. Combustion reactions

$$C + 1/2O_2 \rightarrow CO \qquad \Delta H = -111 MJ/Kmol \quad (1)$$

$$CO + 1/2O_2 \rightarrow CO_2 \qquad \Delta H = -283 MJ/Kmol \quad (2)$$

$$H_2 + 1/2O_2 \rightarrow H_2O \qquad \Delta H = -242 MJ/Kmol \quad (3)$$

2. Boudouard reaction

$$C + CO_2 \rightarrow 2CO \qquad \Delta H = +172 MJ/Kmol \quad (4)$$

3. Water Gas Reaction

$$C + H_2O \leftrightarrow CO + H_2 \qquad \Delta H = +131 MJ/Kmol \quad (5)$$

4. Methanation reaction

$$C + 2H_2 \leftrightarrow CH_4 \qquad \Delta H = -75 MJ/Kmol \quad (6)$$

As proposed by Nagpal [14], fixed and volatile carbon will undergoes carbon combustion, gasification, and volatilization reactions. Ash is assumed to be chemically inert inside the gasifier.

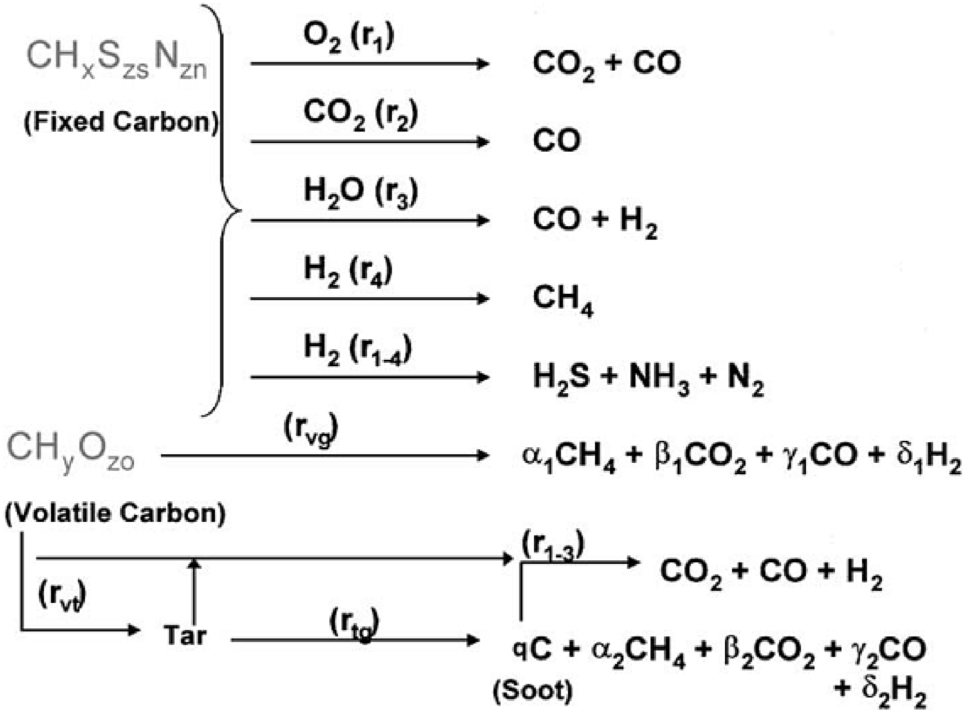


Figure 2.5: Schematic of fixed and volatile carbon combustion, gasification, and volatilization reactions considered in model

2.4. Petcoke

Petroleum coke or petcoke is a byproduct from oil refineries [10]. High carbon content presence in petcoke makes it considered as an attractive feedstock for gasification. Other petcoke properties are high heat content, low moisture, low volatility, high sulfur, low ash, and relatively hard/difficult-to-grind fuel (low Hardgrove Grindability Index or HGI). [13].

Less amount of fuel needed as petcoke has higher heat content compared to coal, approximately 14,000 Btu/lb. Low moisture content inside petcoke is the result of its natural ability to repel excess moisture. Low volatile matter turns out to create flame stability problem but less concern for gasification inside fluidized bed reactor. Low ash handling cost and low boiler operating cost due to low ash content in petcoke which is 1 %. By having lower Hardgrove Grindability Index (HGI), petcoke is said to be softer compared to most coals. Details on the basic petcoke properties are shown in Table 2.1.

Table 2.2: Typical Quality Ranges for Fuel-Grade Petcoke

Characteristic	**Specification**
Heat Content	13,000-15,000 Btu/lb
Moisture	<0.5% to 10%
Volatile matter	About 10 %
Sulfur	3.0% - 7.0 %
Ash	0.1% - 0.3%
Hardgrove Grindability Index (HGI)	30 to 70

CHAPTER 3

3. METHODOLOGY

3.1. Research Methodology

In this chapter, the methodology will be divided into two phases which are the project research phase and the project simulation phase.

3.1.1. Phase 1: Project Research

Literature review on articles and journals had been conducted at this phase. This is crucial for further understanding of the topic. Concept and current technologies used for the process can be read from the literature review works.

3.1.2. Phase 2: Model Simulation

After making some assumptions inside the model, the gasification process will be simulated using the process simulator ASPEN HYSIS. During the simulation process, the variation of operating parameters such as the feed oxygen to coke ratio, steam to coke ratio, and coke flow rates on the gaseous component will be examined.

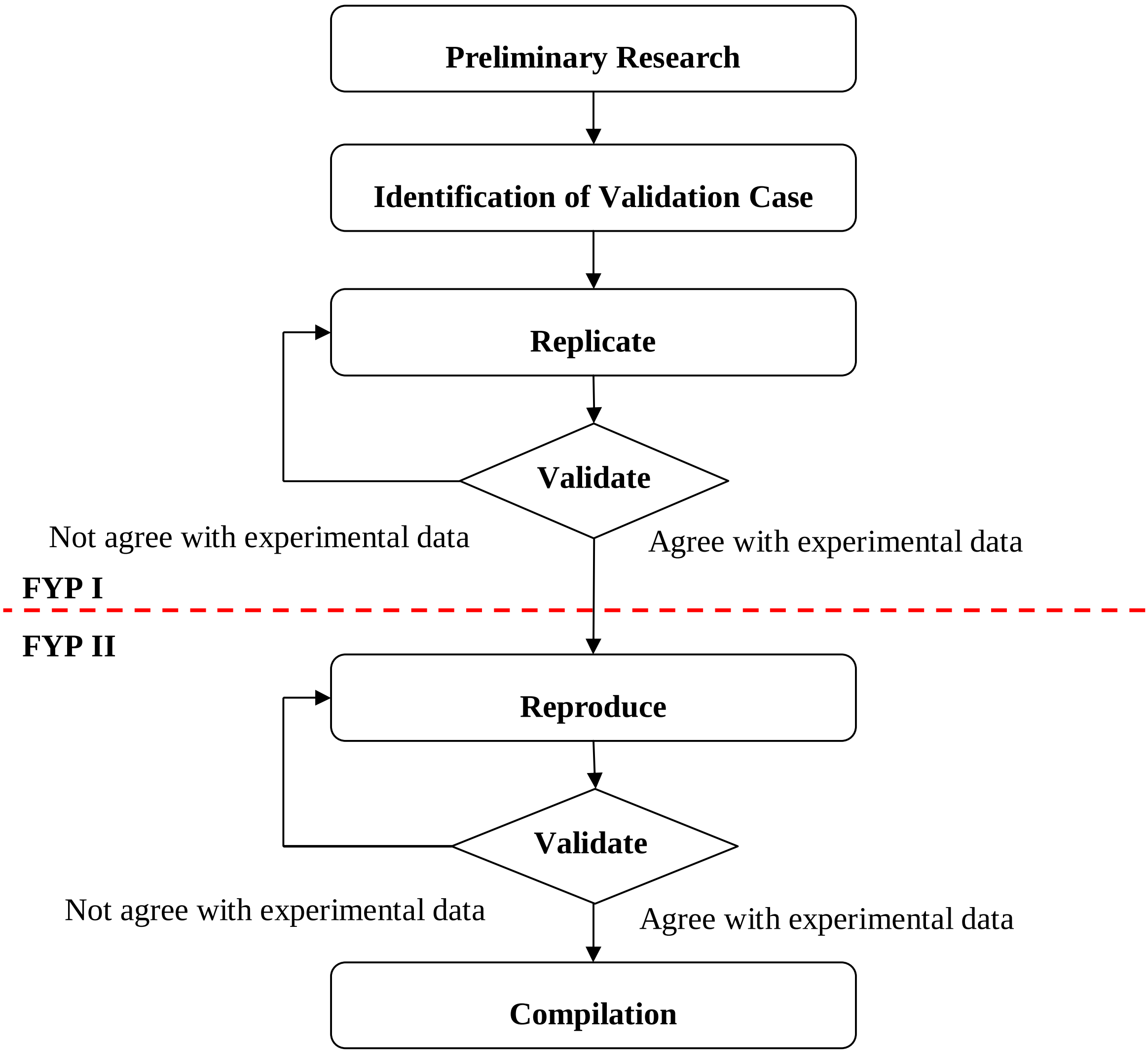
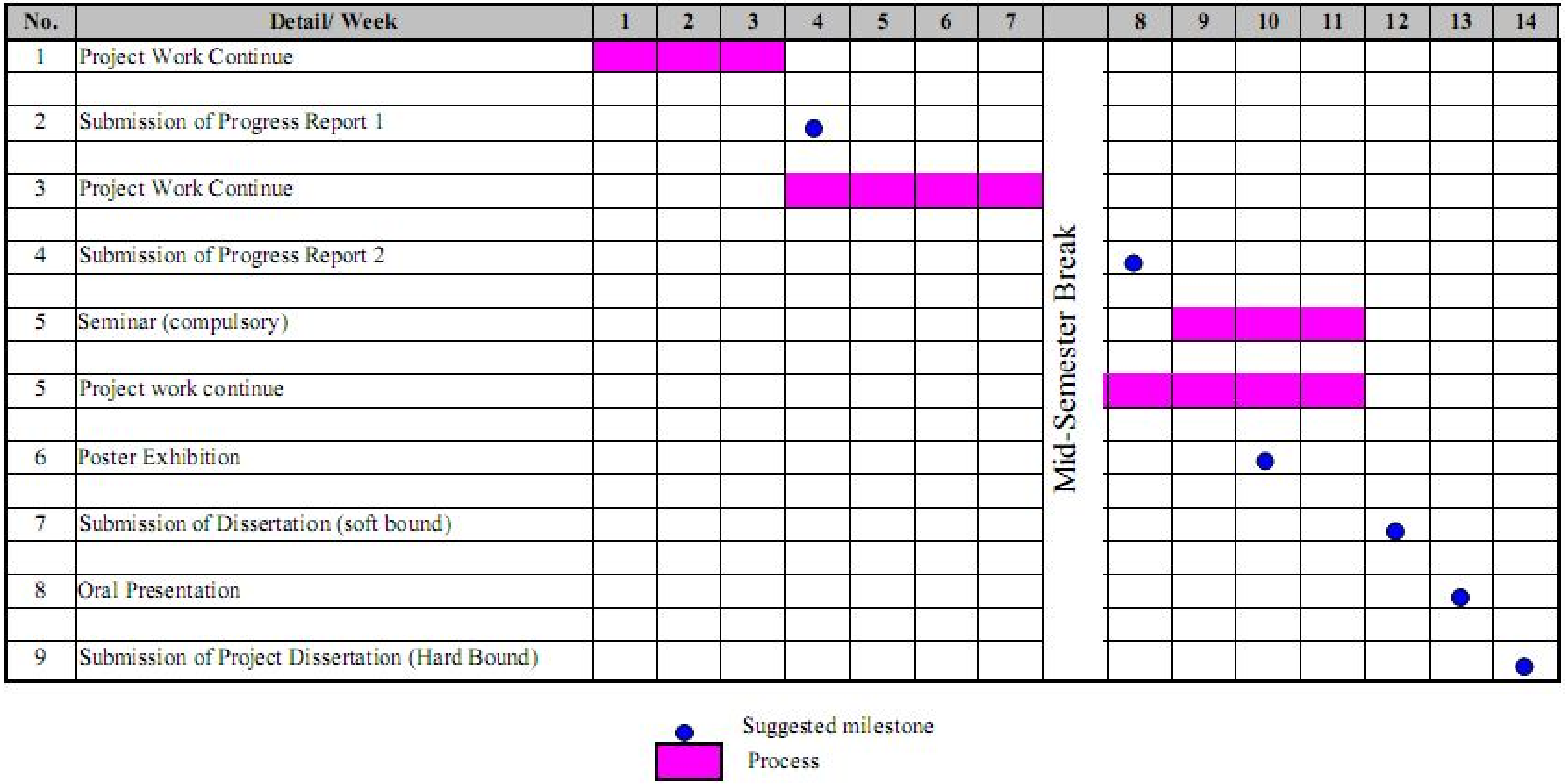


Figure 3.1: Simplified Diagram of Research Methodology in Final Year Project

3.2. Gantt Chart



No.	Detail/ Week	1	2	3	4	5	6	7		8	9	10	11	12	13	14
1	Project Work Continue	■	■	■					Mid-Semester Break							
2	Submission of Progress Report 1				●											
3	Project Work Continue				■	■	■	■								
4	Submission of Progress Report 2									●						
5	Seminar (compulsory)										■	■	■			
5	Project work continue									■	■	■	■			
6	Poster Exhibition											●				
7	Submission of Dissertation (soft bound)													●		
8	Oral Presentation														●	
9	Submission of Project Dissertation (Hard Bound)															●

● Suggested milestone

■ Process

Figure 3.2: Gantt chart

3.3. Tool

ASPEN HYSYS process simulator

3.4. Model Approach

3.4.1. Model Setting

The system to be modeled consists of a gasification system. The following species are presence inside the model: C, H_2, Sulfur, O_2, CO, CO_2, CH_4, N_2, and H_2O. Petcoke composition is from Nagpal et al. [14]. The Peng- Robinson equation of state was applied as the thermodynamic model.

3.4.2. Gasification Model

The combustion and gasification steps were described as Plug Flow Reactor (PFR). Four heterogeneous and one homogeneous reaction have been considered inside the model. The model used kinetics data taken from Nagpal et al. [14] and Goyal et al. [10].

Table 3.1: Kinetics constants of heterogenous reactions involving petcoke

Combustion	$C + O_2 \rightarrow CO+CO_2$	$k=2.128X10_8exp(-158.6/RT)$
Boudouard	$C + CO_2 \rightarrow 2CO$	$k=36.6/pPX10^4exp(-215/RT_E)$
Steam Gasification	$C + H_2O \rightarrow CO+H_2$	$k=7.488X10^5T_Eexp(-240/RT_E)$
Methanation	$C + H_2 \rightarrow CH_4$	$k=2.85X10^{-10} exp (11100/T_E)$

Table 3.2: Kinetics constants of homogenous reaction involving petcoke

Water Gas Shift	$CO + H_2O\rightarrow CO_2+H_2$	$k=2.78X10^3exp(-1510/Tg)$

Table 3.3: Experimental setup parameters used in the simulation

Fluidized bed reactor	
Temperature (^{o}C)	25
Pressure (bar)	1
Flow rate (kg/hr)	461875
Air	
Temperature (^{o}C)	300
Pressure (bar)	1
Flow rate (kg/hr)	14184.96
Steam	
Temperature (^{o}C)	300
Pressure (bar)	1
Flow rate (kg/hr)	13852.5

Table 3.4: Petcoke’s Proximate and Ultimate Analysis

Poximate (%)	
Fixed C	80.6
Volatile C	9.6
Ash	0.5
Ultimate (%)	
C	89.2
H	3.59
N	1.35
O	0.1
S	5.22
Ash	0.5

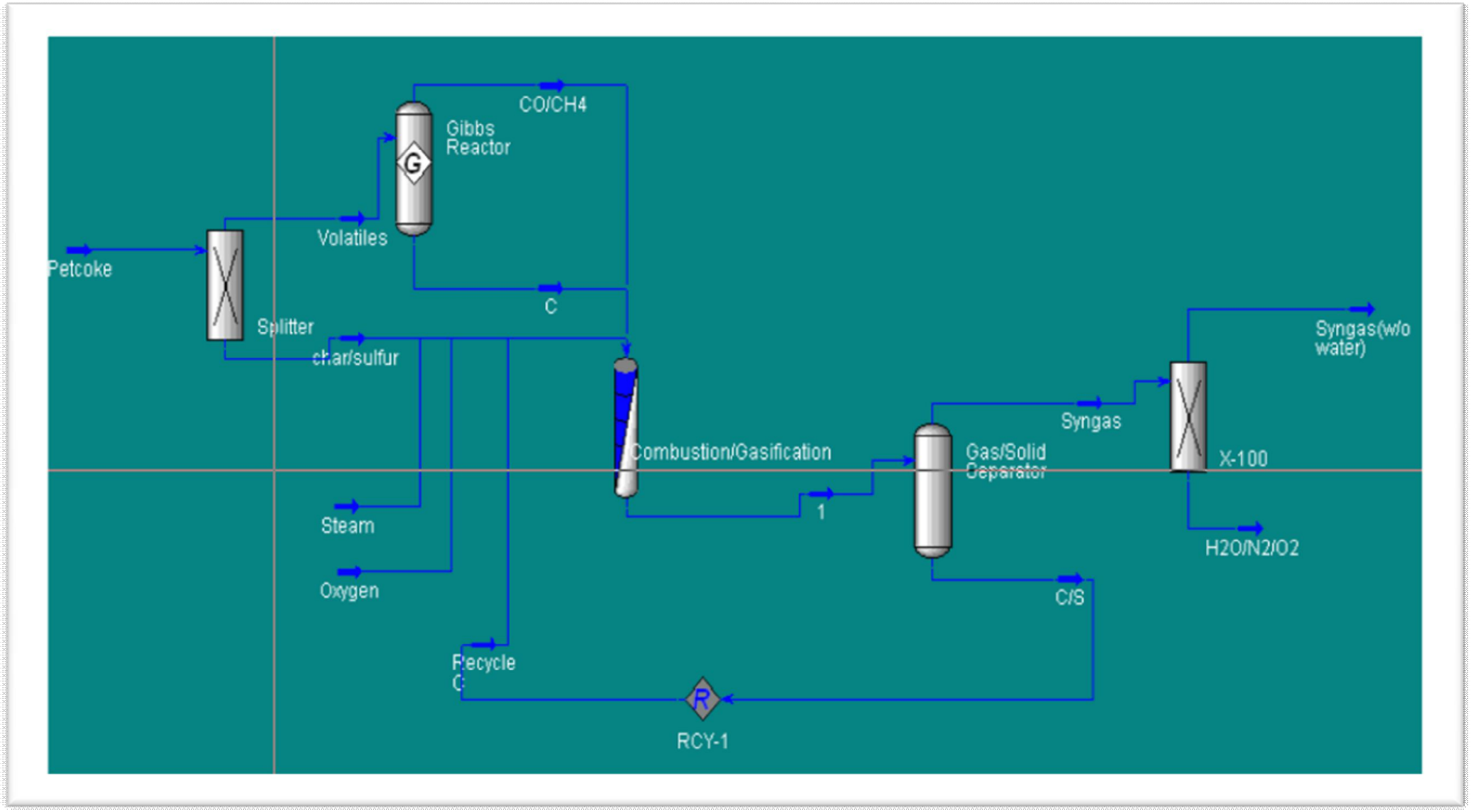


Figure 3.2: Simulation in HYSYS

CHAPTER 4

4. RESULTS AND DISCUSSION

4.1. Data Gathering and Analysis

Table 4.1: Results Composition in HYSYS

Name	**Petcoke**	**Volatiles**	**char/sulfur**	**CO/CH$_4$**	**C**	**Steam**	**Oxygen**
Comp Mole Frac (Carbon)	0.8930	0.9004	0.8920	0.0000	1.0000	0.0000	0.0000
Comp Mole Frac (Hydrogen)	0.0359	0.0912	0.0285	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Oxygen)	0.0010	0.0085	0.0000	0.0000	0.0000	0.0000	1.0000
Comp Mole Frac (S_Rhombic)	0.0701	0.0000	0.0795	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (H_2O)	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
Comp Mole Frac (CO)	0.0000	0.0000	0.0000	0.2708	0.0000	0.0000	0.0000
Comp Mole Frac (CO_2)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Methane)	0.0000	0.0000	0.0000	0.7292	0.0000	0.0000	0.0000
Comp Mole Frac (Nitrogen)	0.0135	0.0000	0.0153	0.0000	0.0000	0.0000	0.0000

Comp Mole Frac (H_2S)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Name	**1**	**Syngas**	**C/S**	**Recycle C**	**Syngas (w/o water)**	**$H_2O/N_2/O_2$**
Comp Mole Frac (Carbon)	1.0000	0.0000	1.0000	1.000	0.0000	0.0000
Comp Mole Frac (Hydrogen)	0.0000	0.0802	0.0000	0.0000	0.8054	0.0000
Comp Mole Frac (Oxygen)	0.0000	0.3293	0.0000	0.0000	0.0000	0.3656
Comp Mole Frac (S_Rhombic)	0.0000	0.0000	0.0000	0.0607	0.0000	0.0000
Comp Mole Frac (H_2O)	0.0000	0.5712	0.0000	0.0000	0.0000	0.6344
Comp Mole Frac (CO)	0.0000	0.0052	0.0000	0.0000	0.0527	0.0000
Comp Mole Frac (CO_2)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Methane)	0.0000	0.0141	0.0000	0.0000	0.1419	0.0000
Comp Mole Frac (Nitrogen)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table 4.2: Material and Energy Balance in HYSYS

Material Streams					
Name	**Petcoke**	**Volatiles**	**char/sulfur**	**CO/CH$_4$**	**C**
Vapour Fraction	0.0369	0.0996	0.0285	1	0
Temperature (^{o}C)	1100	1100	1100	1371	1371
Pressure (kPa)	2800	2800	2800	2800	2800
Molar Flow (kgmole/h)	3531	417.1	3114	26.07	349.4
Mass Flow (kg/h)	46200	4700	41500	502.8	4.200
Liquid Volume Flow (m^3/h)	30.65	3.943	26.71	1.266	2.556
Heat Flow (kJ/h)	183000000	8640000	175000000	-134000	8780000
Name	**Steam**	**Oxygen**	**1**	**Syngas**	**C/S**
Vapour Fraction	1	1	0	1	0
Temperature (^{o}C)	1100	1100	807.2	807.2	807.2
Pressure (kPa)	2800	2800	100	100	100
Molar Flow (kgmole/h)	768.9	443.3	30800000	1346	30800000
Mass Flow (kg/h)	13900	14200	371000000	28800	371000000
Liquid Volume Flow (m^3/h)	13.88	12.47	226000	30.73	226000
Heat Flow (kJ/h)	-154000000	16000000	413000000000	-151000000	413000000000

Name	**Recycle C**	**Syngas (w/o) water**	**$H_2O/N_2/O_2$**
Vapour Fraction	0	1	0
Temperature (^oC)	807.1	807.2	807.2
Pressure (kPa)	100	100	100
Molar Flow (kgmole/h)	30800000	134	1212
Mass Flow (kg/h)	370000000	720.5	28000
Liquid Volume Flow (m^3/h)	226000	4.381	26.35
Heat Flow (kJ/h)	413000000000	1300000	-152000000

4.2 Effect of variation in model parameters towards syngas composition

4.2.1 Effect of Temperature

Temperature variation was aimed mainly at the final composition of the syngas coming out of the gasifier. Here, the compositions of CO and H_2 inside the syngas were been monitored. The temperature range studied is from 700°C until 1100°C.

Table 4.2: Effect of temperature on syngas composition

Temperature (°C)	H_2 (%)	CO (%)	CH_4 (%)
700	79.16	5.64	15.19
800	79.91	5.44	14.65
900	79.32	5.6	15.08
1000	81.66	4.97	13.38
1100	82.6	4.71	12.69

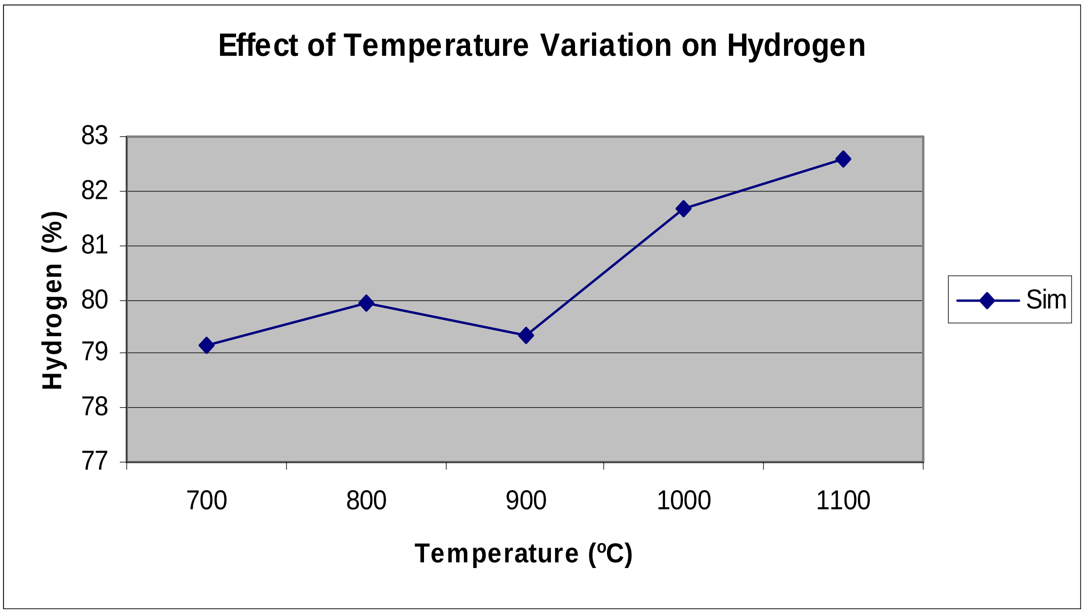


Figure 4.1: Effect of temperature on hydrogen

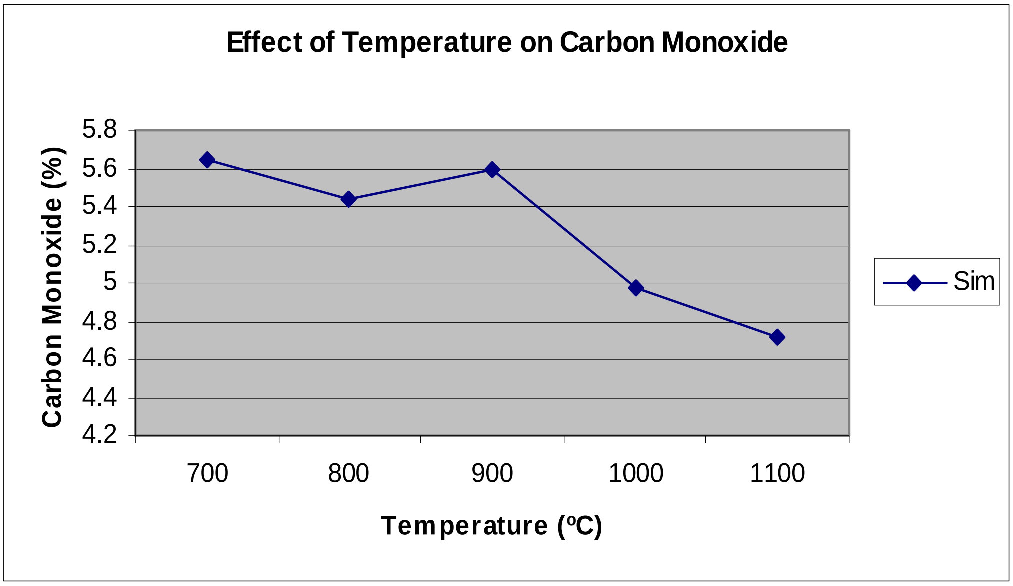


Figure 4.2: Effect of temperature on carbon monoxide

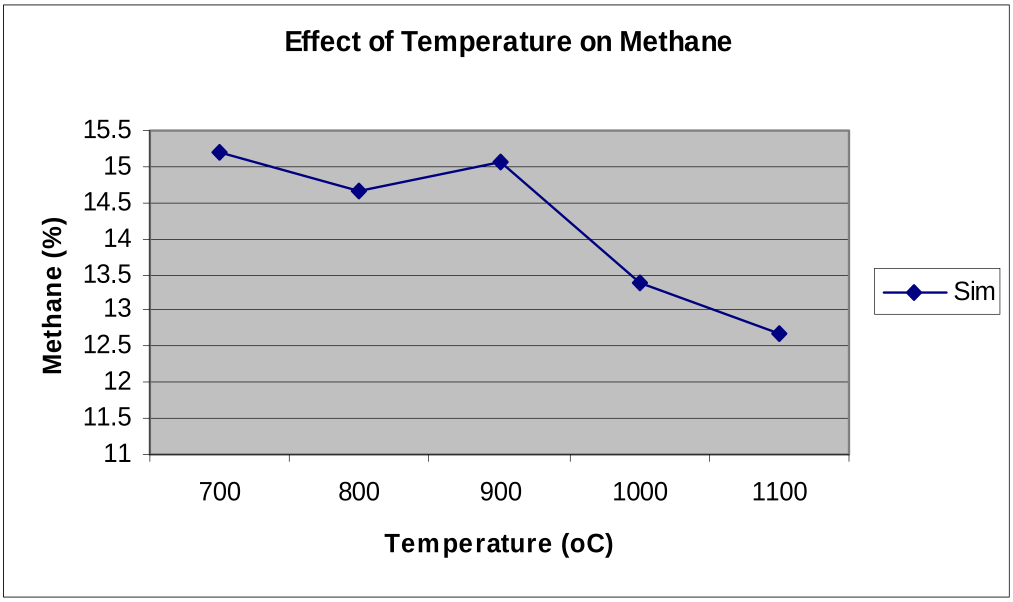


Figure 4.3: Effect of temperature on methane

From figure 4.1, we can see that as the temperature increases, the production of hydrogen will also increase. And less production of carbon dioxide and methane as the temperature increased. This is because higher temperature will increase the carbon conversion. Thus, more petcoke will be converted into hydrogen.

However, Jayakumar [3] in his work states that at very high temperature, the concentration of both carbon dioxide and hydrogen will start to decrease. This is because both carbon dioxide and hydrogen are unstable at high temperatures and will convert into completely combustible products such as carbon dioxide and water if the oxygen supply is sufficient. Besides, as suggested by Rezaiyan et. al [21], higher temperatures will promote gas formation while lower temperatures promote char and tar formation.

Hydrocarbon presence in this simulation is methane as the assumption that homogeneous reactions follow Gibbs equilibrium reaction. From figure 11, methane production reduces with temperature. As agreed by Mehrdokht et al. [4], that at lower temperature, petcoke produces more tar an unburned hydrocarbon which in this case is methane.

4.1.1. Effect of oxygen to coke ratio

Oxygen variation was aimed at maximizing the flowrate of the carbon monoxide and hydrogen mixture and at minimizing the flowrate of the completely combustible products, carbon dioxide and water vapor. Inside the simulation, the range of oxygen to coke ration from (0.1-0.5) had been studied and the results obtained as per figures below.

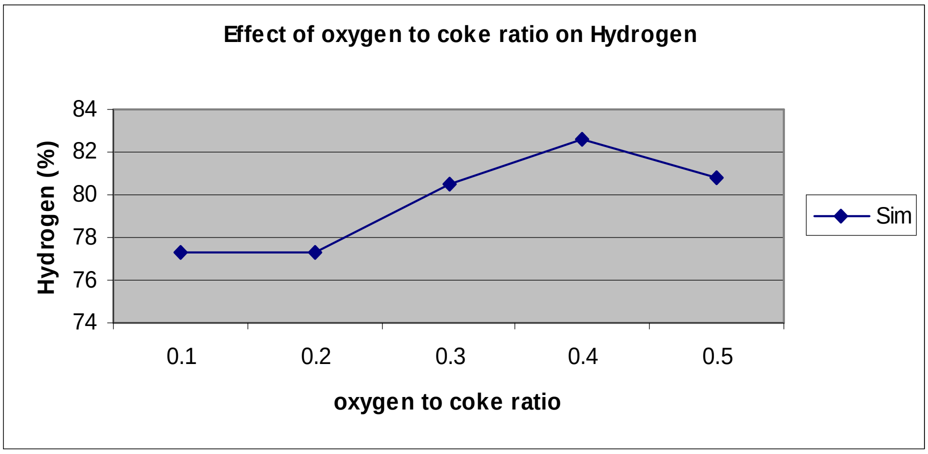


Figure 4.4: Effect of oxygen to coke ratio on hydrogen

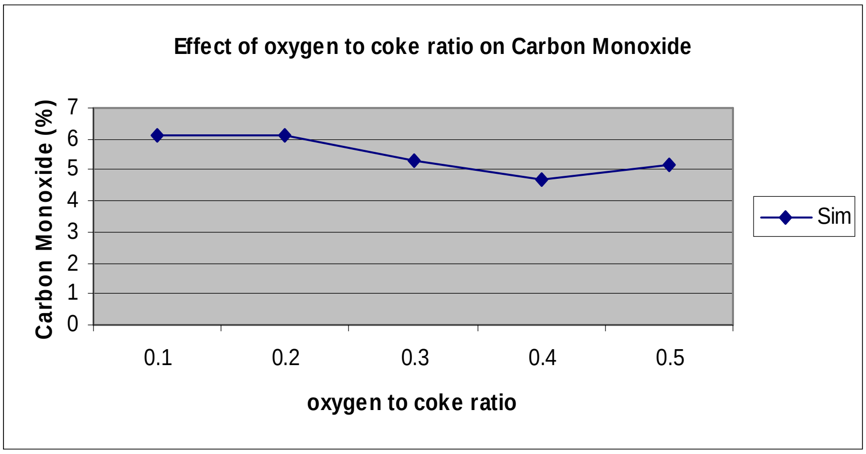


Figure 4.5: Effect of oxygen to coke ratio on carbon dioxide

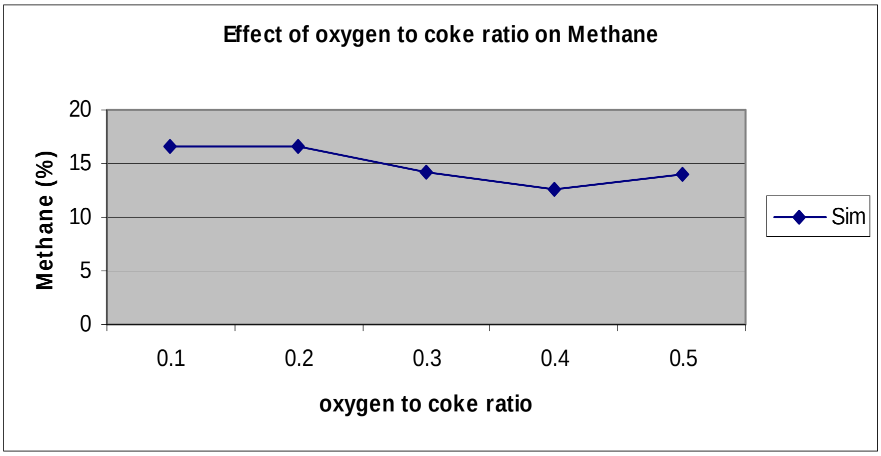


Figure 4.6: Effect of oxygen to coke ratio on methane

From figure 4.4, higher oxygen to coke ratio will result in higher conversion of petcoke. More hydrogen will be produced as the oxygen increases. Besides, less carbon dioxide and hydrogen will be produced as the oxygen to coke ratio increased (figure 4.5 and figure 4.6). This had been highly agreed by S. Nagpal et al. [14] in his works, which states that the CO/H_2 ratio increases with the oxygen to coke ratio. Thus, maximizing the flow rate of carbon monoxide and hydrogen in the syngas stream increases the heat content of the outlet stream. However, at very high oxygen supplied, more carbon dioxide will be produced due to the complete combustion.

4.1.2. Effect of steam to coke ratio

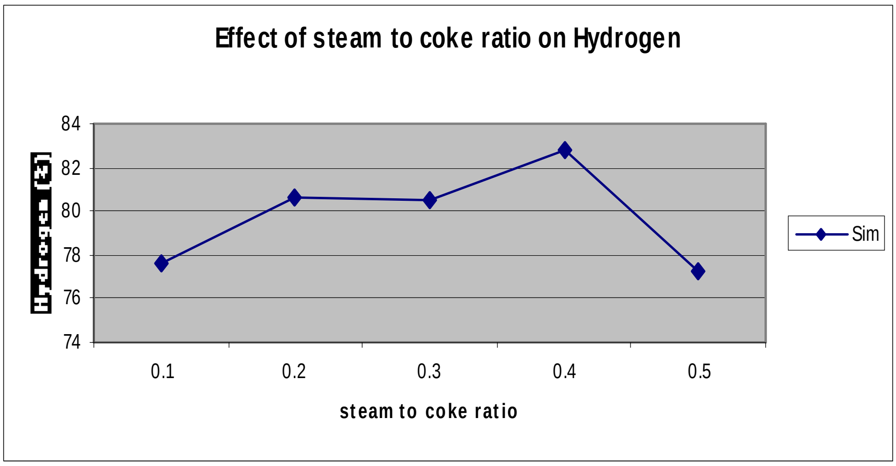


Figure 4.7: Effect of steam to coke ratio on hydrogen

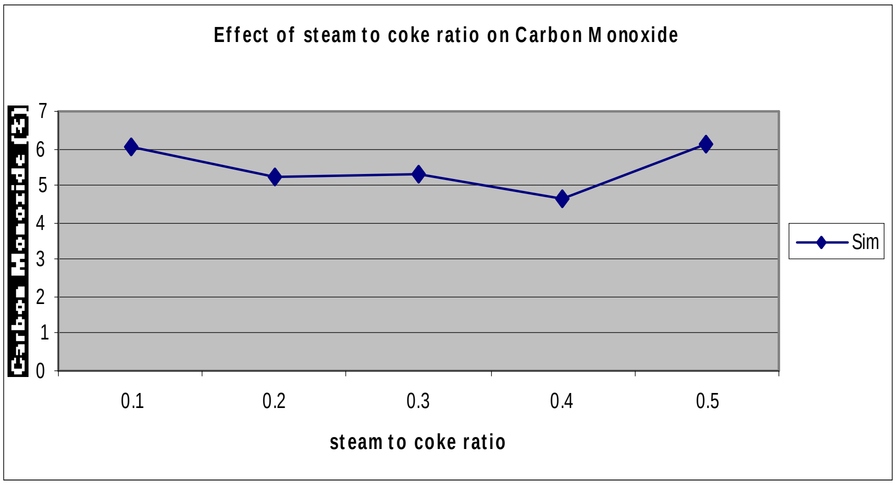


Figure 4.8: Effect of steam to coke ratio on carbon dioxide

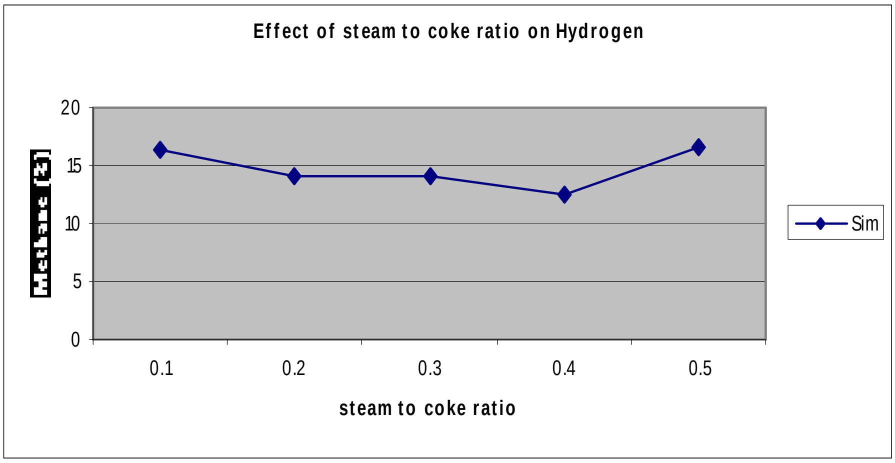


Figure 4.9: Effect of steam to coke ratio on methane

As seen in the figure 4.7, figure 4.8 and figure 4.9, a higher flowrate of steam will increases hydrogen and reduces carbon monoxide and methane composition inside the system. Thus, petcoke conversion is said to be increased as the steam to coke ratio increases. By introducing less steam into the gasification process, the temperature of the process will be reduced and hence increases the formation of tar. As a result, less hydrogen will be produced.

Higher steam to coke ratio fed into the gasification process will result in increase water gas shift (WGS) reaction rate. The water gas shift (WGS) reaction plays an important role in determining the final composition of the gas species and mostly occurring forward to form hydrogen and carbon dioxide until equilibrium is reached. Thus, higher reaction rate will increase the hydrogen and carbon dioxide composition. Later then will participate in the CO_2 gasification reaction to produce more syngas products.

CHAPTER 6

CONCLUSION AND RECOMMENDATION

A model was developed for the gasification of petcoke in a fluidized bed gasifier using the ASPEN HYSYS process simulator. To provide with the gasification model, several ASPEN HYSYS unit operation blocks were combined and where necessary, kinetics expressions were developed using data taken from the literature. Variation on the temperature, oxygen to coke ratio, and steam to coke ratio had been studied in the process simulator. Higher temperature improves the gasification process. More hydrogen is produced as the temperature increase. Increasing both oxygen to coke ratio and steam to coke ratio will result in higher production of hydrogen and reduces both production of carbon monoxide and methane.

However, during conducting the project, there are several problems arise. It is found that fewer works on the petcoke gasification experimental works are available. As a result, data were available for detail comparison with the model. Thus, to validate the model, data from the fluidized bed gasifier is necessary. Currently, PETRONAS and TNB is collaborating in a research work for syngas production located at TNBR, Bangi employing the fluidized bed reactor. Thus, it is recommended to use the data from the experimental works to validate the results from the model.

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