Simulation of Pyrolysis and Gasification of Sub-Bituminous Coal Using Aspen Plus

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***Abstract*— the purpose of this study is to simulate the decomposition process of the coal by pyrolysis process and to simulate the gasification process of the pyrolysed product. Simulation of this process was done in order to transform the coal into synthesis gas. This was done by using pyrolysis and gasification process. Gasification is a process where thermochemical reactions takes place. The coal was transformed by partial oxidation into synthetic gases. In the simulation by using Aspen Plus, the main syngas formed is carbon monoxide, hydrogen and carbon dioxide. These gas are used in electricity generation as a fuel to the turbines. In this project, the rigorous model that was used to simulate the pyrolysis and gasification process is R-Yield and R-Gibbs respectively. R-Gibbs model are used to determine the equilibrium composition of the expected products which involves various kinds of chemical reactions. R-Yield model was used to simulate the decomposition yield of the coal based from the ultimate analysis and proximate analysis obtained from references. The R-Yield model was simulated with the help of FORTRAN code which is needed to calculate the amount of yield. The syngas yield from the gasifier are 85.47% mass. A solid-gas separator was used to simulate the separation of the ashes obtained from the pyrolysis process. The main concern of the process is the cleaning of the gas. The results obtained shows that the cyclone which was used for the solid-gas separation was successfully separated with an efficiency as high as 95%.**

Keywords—Sub-bituminous coal, Pyrolysis, Gasification.

I. Introduction

Pyrolysis and gasification are used in industry in order to convert industrial fuel which may be a regular fossil fuels such as coal, biomass, crude oil and natural gas into a chemical or nuclear energy as heat or to be used for work. Gasification is a process which converts these fuels into syngas which is carbon monoxide, hydrogen and carbon dioxide. Syngas is an intermediate compounds which holds many uses, these production of syngas brings a lot of benefits towards the industry and has opened up a wide variety of research opportunities in renewable energy resources. The main usage of syngas is in the electrical generation which the generation of the electricity is from the power provided from the combustion of the syngas.

It is known that in the generation of electricity and the demand of energy, fossil fuels such as coal, gas and oil are the responsible source of energy being used as the fuel. Coal, compared to the other fuels are the largest source of energy for generation of electricity worldwide. Coal are largely used as a fuel due to its known reliability, affordability, abundance, known energy and safety. Energy produced from coal fired plants is cheaper and more affordable than other energy sources. Since coal is abundant, it is cheaper to produce power using this fuel. Moreover, it is not expensive to extract and mine from coal deposits. Consequently, its price remains low compared to other fuel and energy sources.

In coal fired plant, the most common method being used to utilize these fuels are by using pyrolysis and gasification process. The process chosen for the utilization of coal depends on the rank of a coal. Sub bituminous coal was used as the fuel for its abundancy and its low sulphur content. It is stated that 30% of available coal resources was sub bituminous [7].For the lower rank coal (sub bituminous coal), process of advanced IGCC was used in order to obtain a higher sub bituminous coal utilization, thus resulting a higher power generation efficiency. [7].

The process of processing syngas consist of three main parts, which are the drying part, the gasifier part and the solid removal part. The gasifier part is the process where the coal will undergoes two process which are the pyrolysis of the coal and the gasification of the pyrolysed products.

The coal will be sent to pyrolysis process before undergoes gasification process. The sub bituminous coal were pyrolysed at a low temperature (260 °C) to remove moisture and a portion of volatiles. The resulting char is subsequently fed into an entrained-flow gasifier. The pyrolysis process is an important step for coal gasification since it strongly influences the distribution of volatile products.

For the gasification process, there are three types of reactor which was commonly used for the process. The three most common reactor that were used are the moving bed gasifier, fluidised bed gasifier and entrained flow gasifier. The selection of the reactor depends on the properties and the characteristic of the coal itself. For the sub bituminous coal entrained flow gasifier was selected as it is more suitable for coal that produce low ash content and able to avoid slagging [1].

The process of gasification and pyrolysis of sub bituminous coal were studied to obtain the composition of the product, and the process optimization which are important in order to obtain a better utilization of coal thus increase the efficiency. Since the study are not done practically, a simulation was done by using program. Program modelling software such as Aspen Plus were widely used to simulate the process of carbon conversion.

II. METHODOLOGY

A. Materials

In Victoria, Australia, the usage of brown coal which is a sub bituminous and lignite coal had been widely used and become the major sources for the generation of 85% of the electricity in Australia [1]. The reason why Victoria Brown coal was widely selected is due to the advantages that it gives in industry which is large reserves (high availability),low cost , high reactivity and a low number of ash (less than 3 wt.% on dry basis). Thus brown coal was selected as the material to be chosen in this study.

B. Simulation Model

In this simulation the property package was selected is Ideal property method. The selection of Ideal because the process involved conventional components which are H_2O N_2, O_2 and other gases and these process run at a low pressure. The summarization of flow diagram of pyrolysis and gasification of coal simulation are shown as figure 1:

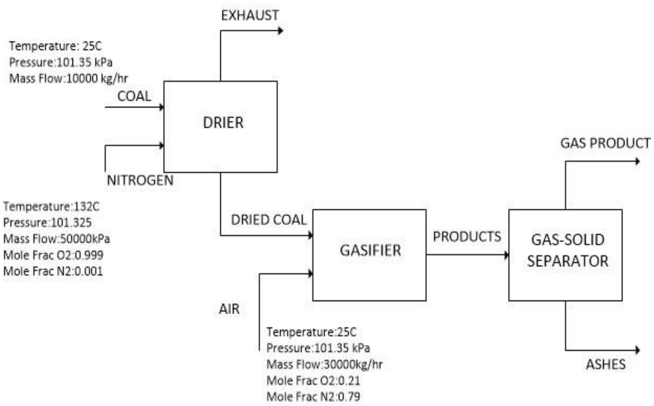

Figure 1: Process Flow of Pyrolysis and Gasification

In order to simulate the drier, an R-Stoic block is being used to models the drying of the coal. It is known that during the process of drying, no chemical reactions are involved, but the conversion of a portion of coal to water need to be performed by using r-stoic because the removal of water of a non-conventional components can only be achieved by using calculation.

In the simulation of pyrolysis using Aspen One, most of the researchers used an Aspen Plus yield reactor (R-Yield) in order to avoid the complex chemical-physical reactions [4]. The pyrolysis process were modelled by using a built-in FORTRAN calculator. The calculation are mainly used to obtain the yield of volatile components via the decomposition into its simpler components which are [C, S, H2, N2, CL2 and O2]. The calculation of these components are based from the proximate analysis of raw feedstock (sub-bituminous coal).

In Aspen Plus, the gasification process was modelled using R-Gibbs reactor. R-Gibbs reactor will restrict chemical equilibrium of specified reactions to simulate gasification. In the simulation the product are obtained by predicting the gasifier output based on the minimization of Gibbs energy [2].

The output of the gasifier mainly contains a mixture of solids and gas. The solids are mainly consists of ashes and need to be removed from the gas. Before being introduced to a gas-solid separator the stream output of the gasifier needs to be reduced it temperature as the temperature stream output are fairly high(1800^oC). After the temperature had been reduced by using a cooler, the stream will now will be fed in into the cyclone. The description of Aspen Plus unit operational models are tabulated in table 1:

Table 1: Representatives unit operations used in simulation

Unit Operation	Aspen Plus Model	Specification
Coal drying	R-Stoic	Rigorous simulation of coal moisture drying
Coal Pyrolysis	R-Yield	Simplified simulation of coal pyrolysis, the yield components based on ultimate analysis
Coal Gasification	R-Gibbs	Gibbs-free energy reactor, restricts chemical equilibrium of specified reactions to simulate gasification
Cyclone		Use of cyclone to separate ash

C. Assumptions

During the simulation of pyrolysis and gasification process, there are several assumptions that were done in order to successfully simulate the process, the basic assumptions in the model are as follows:

1. The system at steady state and Isothermal.
2. The ash formed is considered as inert and does not take part in the reaction process.
3. Char consists only fixed carbon.
4. The pressure loss are not taken into account in the simulation.

D. Data needed for simulation

During the introduction of the coal stream, SULFANAL, ULTANAL and PROXANAL are the terms that were used by Aspen Plus to define the proximate and ultimate analysis. The rules need to be followed as to avoid any error from occurring. After defining the components, the enthalpy and density model for the coal need to be defined. In this simulation which involves a non-conventional components, the HCOALGEN and DCOALIGHT are used. This models includes the number of empirical correlations for heat of combustion and the heat capacity. Table 2 and 3 show the data used for the coal [1]:

Table2: Proximate analysis for three types of brown coal

Proximate, wt.% dried basis				
	M	FC	VM	ASH
VBC	65.2	46.82	50.57	2.61
CHL	26.7	38.7	44.2	17.1
BLK	3.3	41.49	24.66	33.85

(*VBC: Victorian brown coal, CHL: Chinese coal, BLK: Black coal, M: moisture content, FC: Fixed Carbon, VM: Volatile matter)*

Table3: Ultimate analysis for three types of brown coal

Ultimate wt.% dried basis					
	C	H	O	N	S
VBC	67.94	4.63	24.08	0.45	0.29
CHL	59.8	3.8	18.06	0.77	0.47
BLK	48.64	3.65	12.36	0.81	0.69

(*VBC: Victorian brown coal, CHL: Chinese coal, BLK: Black coal, M: moisture content, FC: Fixed Carbon, VM: Volatile matter)*

During the process of gasification, the reactions involved in the process need to be known. The reactions involved in the gasifier are shown in Table 4.

Table4: Equilibrium reactions in the gasifier

Reaction	
$C + 0.5O_2 \rightarrow CO$	(1)
$C + CO_2 \rightarrow 2CO$	(2)
$C + H_2O \rightarrow CO + H_2$	(3)
$CO + 0.5 \rightarrow CO_2$	(4)
$H_2 + 0.5O_2 \rightarrow H_2O$	(5)
$CO + H_2O \rightarrow CO_2 + H_2$	(6)
$CO + 3H_2 \rightarrow CH_4 + H_2O$	(7)
$S + O_2 \rightarrow SO_2$	(8)
$H_2 + Cl_2 \rightarrow 2HCl$	(9)

III. RESULTS AND DISCUSSION

A. Overall Aspen Plus Simulation Diagram

The process was simulated by using Aspen Plus, and the results are shown as in figure 2:

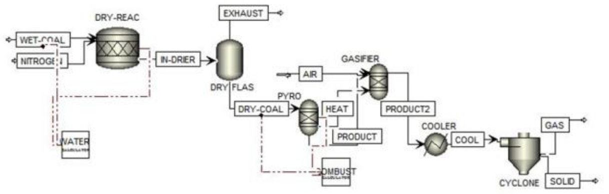

Figure 2: Simulation of Coal Pyrolysis and Gasification

The figure 2 shows the results from the simulation, the data shows the simulation was done successfully, the data collected were discussed for the main unit which are the pyrolysis and gasification unit.

B. Pyrolysis

The result obtained from the simulation are shown in table 5 and 6. The simulation was done by using unit kg/hr. The results obtained shows that the decomposition of coal are successfully simulated by using the R-Yield block. The decomposition of the coal are being done by the use of FORTRAN calculator.

Table5: Pyrolysis operating condition

Pyrolysis Process			
Stream ID	Unit	Product	Dry-Coal
Temperature	C	260.000	40.000
Pressure	Kpa	101.350	101.350
Mass V-Fraction		0.308	1.000
Mass S-Fraction		0.692	0.000

Table 6: Pyrolysis Process

Pyrolysis Process(Mass Flowrate)			
Component ID	Unit	Product	Dry-Coal
H_2O	kg/hr	814.440	0.000
N_2	kg/hr	55.708	0.000
O_2	kg/hr	1323.798	0.000
S	kg/hr	34.451	8144.444
H_2	kg/hr	278.450	0.000
CL_2	kg/hr	0.733	0.000
ASH	kg/hr	1253.430	0.000
C	kg/hr	4383.34	0.000

In pyrolysis process, there are three main components that are expected to be formed from the process, these components are char, coal gases and liquids. Char are defined as un-distillable material which remains in the form of solids and assumed to only consist of fixed carbon in this study. Coal gaseous are the gas that are lighter than C_6 such as carbon monoxide, methane, hydrogen gas, water and carbon dioxide. The liquids are the components that have a molar mass higher than C_6. From the results obtained the general equation of pyrolysis of coal are defined as:

$$\text{DRY COAL} \rightarrow \text{CHAR} + \text{COAL GASES} + \text{LIQUID} \quad (10)$$

A manual calculation was done by using the ultimate analysis as the yield. It is found that the calculations that were done using FORTRAN and manually are similar. A comparison between the simulated results and the results obtained from the pilot lab experiment [2] are tabulated in table 7.

Table 7: Comparison of experiment data and the simulation results

	Mass fraction %		
Products	Coal gases	Coal Solids	Water
Experiment	55.47	15.91	28.61
Simulation	20.37	68.82	10.81

It is needed to be taken into the consideration that the data from the experiment are taken from various resources and the experiment are operating in a different operating conditions. The operating conditions differs such as the gasifier pressure, temperature and the coal type.

C. Coal Gasification Product

The results shows the specified reactions involved in the gasifier. The gaseous components such as the carbon monoxide, the carbon dioxide and the hydrogen were successfully produced which proved the chemical equations provided in table4. Table 8 and 9 shows the composition and operating condition of stream involved in the gasifier.

Table 8: Gasification process operating condition

Gasification Process			
Stream ID	Unit	Product	Product2
Temperature	C	260.000	1635.000
Pressure	Kpa	101.350	101.350
Mass V-Fraction		0.308	0.987
Mass S-Fraction		0.692	0.013

Table9: Gasification Process Stream

Gasifier Process Streams(Mass Flowrate)			
Component ID	Unit	Product	Product2
H_2O	lb/hr	814.44	2831.32
N_2	kg/hr	55.708	30739.00
O_2	kg/hr	1323.798	38.212
S	kg/hr	34.451	0.188
H_2	kg/hr	278.450	52.835
CL_2	kg/hr	0.733	0.000
ASH	kg/hr	1253.430	1253.430
SO_2	kg/hr	0.000	68.455
CO	kg/hr	0.000	5078.610
CO_2	kg/hr	0.000	8081.620
HCL	kg/hr	0.000	0.754.000

The results from the simulation will then be compared with the industrial data [3]. The comparison of the data are mainly focused on the syngas produced from the gasifier. The comparison of data are tabulated in table 10:

Table 10: Comparison of industrial gasification data and simulation results

Mass fraction %				
Syngas	CO	CO_2	H_2	Total
Industrial data	15.65	31.21	38.61	85.47
Simulation	31.44	50.00	0.3	81.74

The data shows that the mass of H_2 syngas produced from the simulated gasifier are much lower than the value of H_2 produced from the industrial gasifier. The difference of the amount of H_2 produced was mainly due to the amount of air being fed into the gasifier. A test run was done and the volume of the H_2 increased as the amount of air fed in are reduced. The overall syngas produced from simulation and industrial data are similar which are 85.47% and 81.74% respectively.

IV. Conclusion

Conclusion was made based on the objective of the research done. The simulation was successfully performed, and the process of the coal gasification and pyrolysis consist of three main operations which are the coal drying, gasifier and the solid removal. The moisture content of the coal managed to be removed from 26.7wt% to 10wt%. The pyrolysis simulation of the coal able to simulate the decomposition of the coal to its constituent elements based on its ultimate analysis. The decomposition of the products consists of 20.37% of coal gas, 68.82% of coal solids and 10.81% of water. The results obtained from the simulation are compared with the data obtained from research. The type of reactions occurred are able to be identified and the syngas were able to be formed. The syngas formed from the gasifier is 85.47% wt. The solid separations shows that the removal of solid are as high as 95% efficiency.

Acknowledgment

For the past months, I was able to achieve a better understanding and the ability to complete the project. During the process of the study, I have communicate with various kind of people and I am really grateful for them for enabling me to complete my project. The things that I have learnt is on how to simulate a process using another Aspen product, which is Aspen Plus. Instead of using Aspen Hysys, Aspen Plus was used to run the simulation. I believe that being able to understand on how to use a two different software will be beneficial in the future. My upmost gratitude goes to my supervisor, Dr. Noor Fitrah Abu Bakar who had always support and guide me through my research and many thanks to my previous supervisor, Miss Siti Norazian Ismail. Both of them had truly inspired me to be successful in this field and set great examples for me to keep learning from failures and never give up.

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