Simulation of Coal Gasification Process using ASPEN PLUS

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Abstract-- **Gasification is an important route for conversion of coal or solid wastes materials to useful gaseous products for direct firing in thermal applications and as well as raw gas for production of fuels or chemicals. Gasification with O_2, H_2O, CO_2 and H_2 produces combustibles such as CH_4 and CO/H_2 mixtures for use as gaseous fuels or chemical feed stocks. Among the coal-gasification processes, the fluidized-bed process with inherent advantages of high heat transfer and easy handling of solids is a natural choice. Coal gasification with O_2 and H_2O in a fluidized-bed reactor involves pyrolysis, combustion and steam gasification. Gasification in fluidized bed offers advantages, since fluidized beds are capable of being scaled up to medium and large scale, overcoming limitations found in smaller scale, fixed-bed designs. This paper gives overview of the coal gasification process. Simulation of coal gasification process was carried out using Aspen Plus. Effect of various parameters like steam to coal ratio and oxygen flow rate effects on product gas composition were studied.**
Keywords— **Aspen Plus Simulation, Coal Gasification, Combustion, Fischer-Tropsch, Fluidized Bed**

I. INTRODUCTION

Energy demand increases day by day at national or international level. In view of limited liquid fuel in terms of crude oil reserves, researchers are attracted towards Fisher Tropsch reaction. Out of many reactors FBR (Fluidized Bed Reactor) has shown better performance to removal/addition of the heat. FT synthesis process provides complete range of fuels produced by coal gasification. Large numbers of researchers are working in this field.

A fluidization phenomenon is highly complicated and reaction in fluidized bed reactor is another challenge. To understand and predict the composition of the products produced by fluidized bed reactor at best possible operating conditions is desired. This paper describes the coal gasification phenomena and simulation of coal gasification was carried out using Aspen Plus simulator.
Sotudeh-Gharebaagh at al developed a comprehensive model for the combustion of coal in a circulating fluidized bed combustor (CFBC). The proposed model integrates hydrodynamic parameters, reaction model and kinetic subroutines necessary to simulate coal combustion in a CFBC. Kinetic expressions were developed for the char combustion rates The reaction model, which considers only the important steps of coal combustion, was simulated using

four ASPEN PLUS reactor models and several subroutines.[1]

Yong kim at al carried out a simulation study on gas-to-liquid (natural gas to Fischer–Tropsch synthetic fuel) in order to find optimum reaction conditions for maximum production of synthetic fuel. Aspen HYSYS software was used for simulation. Optimum reaction conditions for FTS unit were determined by changing reaction variable such as temperature.[2]

II. COAL GASIFICATION

Coal gasification is the process of reacting coal with oxygen, steam, and carbon dioxide to form a product gas containing hydrogen and carbon monoxide. Gasification is essentially incomplete combustion. [3]
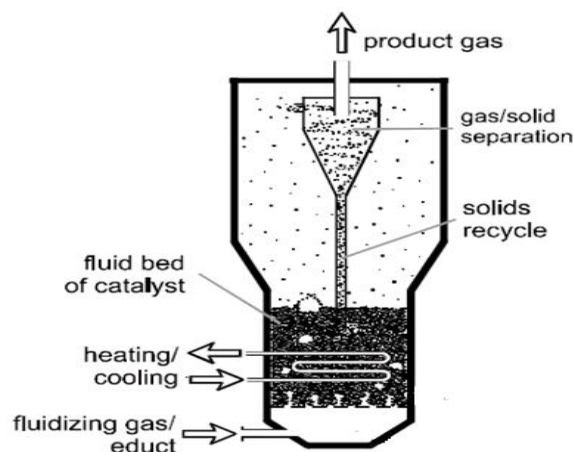

Fig. 1. Fluidized Bed Reactor [3]

Gasification refers to a group of processes which highlight the conversion of solid or liquid fuels into a combustible gas in presence or absence of a gasification agent. It is normally carried out by reacting fuel such as coal, biomass, oil or coke with a minimal amount of oxygen often in combination with steam. The heat liberated from the exothermic reactions of fuel and oxygen maintains the gasifier at the operating temperature and drives the endothermic gasification reactions taking place inside the gasifier. We can use steam as the gasifying agent only if we can provide an external source of heat that drags the endothermic reactions forward. The concern for climatic variations has triggered the interest in gasification making fluidized bed gasifiers as one the popular options, occupying nearly 20% of their market. [4]

Gasification definitely has certain important advantages over direct combustion. When the fuel is processed, the

volume of gas obtained from gasification is significantly less as compared to that of combustion. The reduced volume of gas needs smaller equipment which results in reduced costs. Gasification definitely is an attractive option for remote locations. However one of the important shortcomings of gasification involves the reduced carbon conversion efficiency due to which a certain part of the fuel energy remains in the char. [9]

Advantages of Fluidized Bed Gasification

- Air to fuel ratio can changed which also helps to control the bed temperature.
- Fluidized bed gasifiers are more tolerant to variation in feedstock as compared to other types of gasifiers.
- They maintain uniform radial temperature profiles and avoid slagging problems.
- Higher throughput of fuel as compared to other gasifiers.
- Improved mass and heat transfer from fuel.
- High heating value.
- Reduced char. [3]

Disadvantages of Fluidized Bed Gasification

- Oxidizing conditions are created when oxygen diffuses from bubble to the emulsion phase thereby reducing the gasification efficiency.
- Losses occurring due to particle entrainment. [3]

In a gasifier, coal undergoes a series of chemical and physical changes.
(1) Coal Drying
(2) Devolatilization or Pyrolysis
(3) Combustion
(4) Char Gasification

(1) Coal Drying

As the coal is heated most of the moisture is driven out when the particle temperature is ~105°C. Drying is a rapid process and can be essentially complete when the temperature reaches 300°C depending on the type of coal and heating method used.

(2) Devolatilization or Pyrolysis

Devolatilization or Pyrolysis accounts for a large percentage coal weight loss and occurs rapidly during the initial stages of coal heat up. During this process, the labile bonds between the aromatic clusters in coal are cleaved, generating fragments of molecular weight much smaller than coal. Fragments with low molecular weights vaporize and escape from the coal particle to constitute light gases and tar. The fragments with high molecular weight, and hence low vapor pressures, remain in the coal under typical devolatilization conditions until they reattach to the char

lattice. The solid product left over from devolatilization is char. [2]

(3) Combustion

Char in an oxygen atmosphere undergoes combustion. In gasifiers partial combustion occurs in an oxygen-deficient, or reducing, atmosphere. Gasifiers use 30–50 % of the oxygen theoretically required for complete combustion to carbon dioxide and water. Carbon monoxide and hydrogen are the principal products, and only a fraction of the carbon in the coal is oxidized completely to carbon dioxide. The combustion reaction is written in a general form as follows. where λ varies from 0 (pure CO_2 product) to 1 (pure CO product). The value of λ depends upon the gasification conditions and is usually close to 1.

$$(1+\lambda)C + O_2 \rightarrow 2\lambda CO + (1-\lambda)CO_2$$
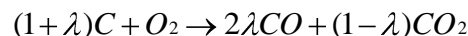
The heat released by the partial combustion provides the bulk of the energy necessary to drive the endothermic gasification reactions.

(4) Char Gasification

The oxygen is rapidly consumed in the combustion zone, which occupies a small volume of the reactor. Further conversion of char occurs through the much slower, reversible gasification reactions with CO_2, H_2O, and H_2.

$$C + CO_2 \rightarrow 2CO$$
$$C + H_2O \rightarrow CO + H_2$$
$$C + 2H_2 \rightarrow CH_4$$
$$CO + H_2O \rightarrow CO_2 + H_2$$
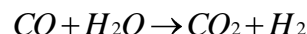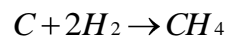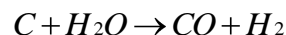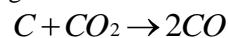
III. FISCHER TROPSCH SYNTHESIS

Synthesis gas produced from coal gasification or from natural gas by partial oxidation or steam reforming can be converted into a variety of transportation fuels, such as gasoline, aviation turbine fuel and diesel fuel. The Fischer-Tropsch process that converts synthesis gas into largely aliphatic hydrocarbons over an iron or cobalt catalyst is widely used for this application. The process was operated successfully in Germany during World War II and is used commercially at the Sasol plants in South Africa. [6]

Fischer Tropsch Synthesis

The Fischer-Tropsch (FT) process is one of the advanced biofuel conversion technologies that comprise gasification of feedstocks, cleaning and conditioning of the produced synthesis gas, and subsequent synthesis to liquid (or gaseous) biofuels. [8]
The Fischer-Tropsch synthesis is extremely interesting because syngas derived from coal can produce liquid transportation fuels such as gasoline (C_5-C_{12}) and diesel (C_{12}-C_{20}). Typical operating pressures for FT synthesis are 15–40

bar, while two temperature modes can be distinguished: high temperature Fischer–Tropsch (300–350°C) and low temperature Fischer–Tropsch synthesis (200–260°C). [7,12]
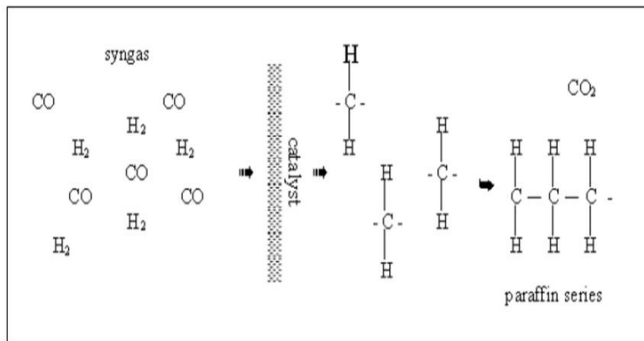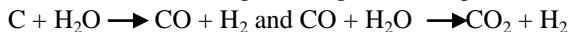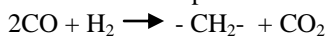

Fig. 2. Fischer Tropsch Reaction [4]

Coal is burned to produce the carbon monoxide and steam reacting with hot coal disassociates to produce hydrogen, as shown in the following "water gas shift" equations:

$C + H_2O \longrightarrow CO + H_2$ and $CO + H_2O \longrightarrow CO_2 + H_2$

Fischer-Tropsch synthesis occurs through two simultaneous reactions promoted by the contact of CO and H_2 with a catalyst:

$2H_2 + CO \longrightarrow -CH_2- + H_2O$ and $CO + H_2O \longrightarrow CO_2 + H_2$
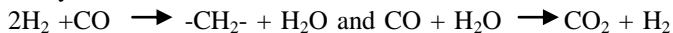
which can be simplified as:

$2CO + H_2 \longrightarrow -CH_2- + CO_2$

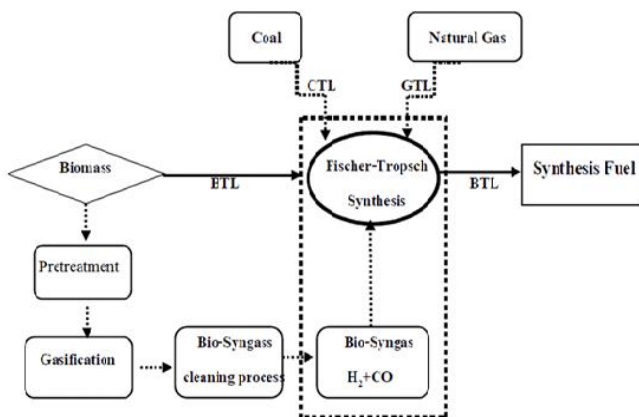Following diagram represents the Coal-to-Liquid (CTL) process.

Fig. 3. Coal To Liquid (CTL) Process [4]

IV. SIMULATION STUDY

The models of the processes considered are developed using Aspen Plus as the process simulator. The different stages considered in ASPEN PLUS simulation, in order to show the overall gasification process, are decomposition of the feed, volatile reactions, char gasification, and gas–solid separation.

[6]

The following assumptions were considered in modeling the gasification process:
- Process is steady state and isothermal
- Coal devolatilization takes place instantaneously and volatile products mainly consist of H_2, CO, CO_2, CH_4, and H_2O
- Char only contains carbon and ash

Coal Decomposition

The ASPEN PLUS yield reactor, RYIELD, is used to simulate the decomposition of the feed. In this step, coal is converted into its constituting components including carbon, hydrogen, oxygen, sulfur, nitrogen, and ash, by specifying the yield distribution according to the ultimate analysis. [8, 10].

Volatile Reactions

The ASPEN PLUS Gibbs reactor, RGIBBS, is used for volatile combustion, in conformity with the assumption that volatile reactions follow the Gibbs equilibrium. mass consists of mainly C, H, N, O, S, Cl, ash, and moisture. Carbon will partly constitute the gas phase, which takes part in devolatilization, and the remaining carbon comprises part of the solid phase (char) and subsequently results in char gasification.

A SEPARATION COLUMN model is used before the RGIBBS reactor to separate the volatile materials and solids in order to perform the volatile reactions. The amount of volatile material can be specified from the coal approximate analysis. Also considering the assumption that char contains only carbon and ash, the amount of carbon in the volatile portion can be calculated by deducting the total amount of carbon in char from the total carbon in coal.

Char Gasification

The ASPEN PLUS stoichiometric reactor, RSTOIC, performs char gasification by specifying the gasification reactions. [8,9,10]
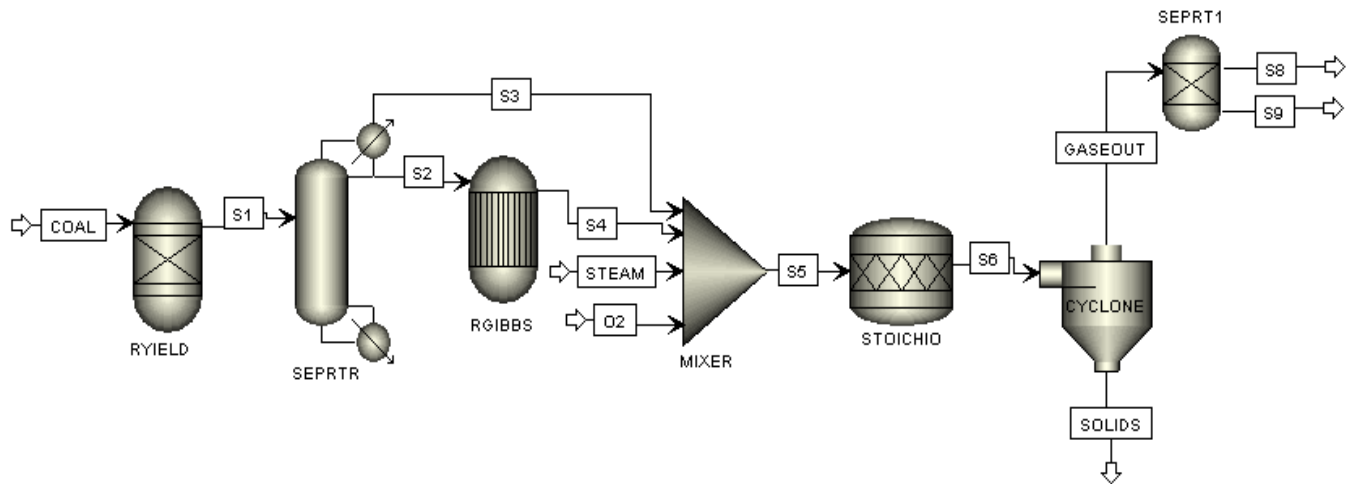
Fig. 4. Simulated Flow sheet of Fluidized Bed Coal Gasification Process

Table 1. Coal composition defined in Aspen Plus

Proximate Analysis	% weight	Ultimate Analysis	% mass
Water	2.2	C	83.8
VM	37.2	N	2
FC	51.3	O	8.4
Ash	13.8	H	4.8
		S	1

Tables 1 and 2 show feed material i.e. coal composition and experimental setup parameters used in the simulation.

Table 2. Experimental Setup Parameters

Parameters	Value
Fluidized bed reactor	
Temperature (^{o}C)	1545
Pressure (bar)	30
Oxygen	
Temperature (^{o}C)	65
Flow rate(kg/h)	10
Steam	
Temperature (^{o}C)	200
Flow rate (kg/h)	5

V. RESULTS AND DISCUSSION

Product Formation

In the Stoichiometric reactor, char gasification will take place. The principal product is synthesis gas i.e. H_2 and CO along with the other components like H_2O, N_2, S, SO_2, SO_3, Cl_2, HCl, CO_2,CH_4 and ash which needs to be separated.

The stream is the outlet stream of the RSTOIC i.e. stream S6. The mass flow rates of all these components are shown in the Table 3.

Table 3. Reactor Outlet Stream S6 Result

Components	Mass Flow rate (kg/hr)
H_2O	3.6
N_2	10.8
S	7.2
SO_2	3.6
H_2	46.8
HCl	10.8
CO	86.4
CO_2	10.8
CH_4	3.6
ASH	21.6

After the product formation, the components generated are in the gas phase and solid phase. So in order to separate these two phases CYCLONE SEPARATOR is provided which will separate the gases which is represented by the stream GASOUT and solids which is represented by the stream SOLIDS from the reactor outlet stream.

Since our principal product is only synthesis gas (H_2 and CO), so a simple SEPARATOR is provided which will separate the other gaseous products which is shown by stream S8 and stream S9 contains only H_2 and CO which can be used for the Fischer-Tropsch Synthesis to produce different synthetic fuels for the next stage.

Table 4 represents the mass flow rates of each component for each stream.

Table 4 Stream Flow rates results

Stream	S1	S2	S3	S4	S5
Components Mass flow rate(kg/sec)					
H_2O	0.012	0.012		<0.001	0.002
N_2	0.003	0.003		0.003	0.003
O2	0.003	0.003			0.003
S	0.003	0.003		Trace	Trace
H_2	0.012	0.009	0.003	0.01	0.013
Cl_2	0.003	0.003		Trace	Trace
C	0.018	0.018			
Ash	0.006	0.006			
CO				0.023	0.023

Simulation Model Analysis

Effect of Variation of Steam Flow (at lower flow rates and higher steam to coal ratios) on Product Gas Composition

Oxygen Flow rate = 10 kg/hr

Coal Flow rate = 5 kg/hr

Steam Flow rate = 5 kg/hr

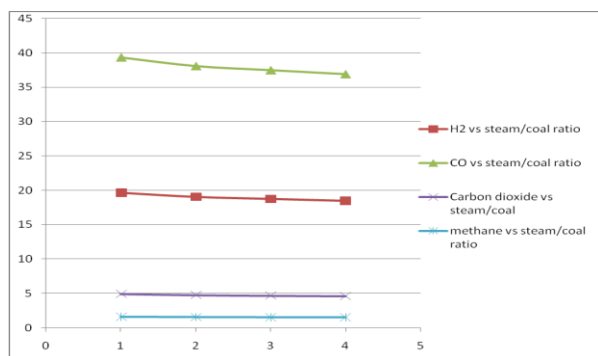The variation of steam flow rate on product gas composition is shown in the figure 5.

Figure 5. Plot of product gas composition versus steam to coal ratio

A decreasing trend in the product gas composition of all the constituents is observed but the decreasing effect is much significant when comparatively higher values of steam are used.

Effect of oxygen flow rate on Product Gas Composition

The effect of oxygen flow rate on the product gas composition is shown in the figure 6.
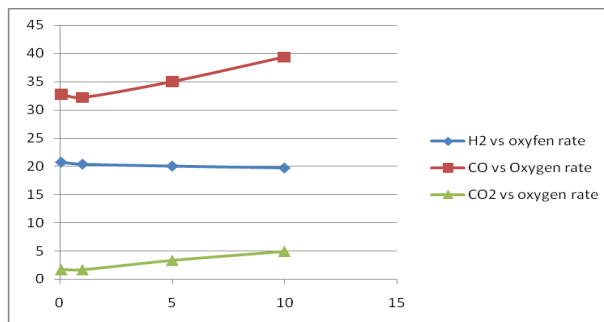

Figure 6. Plot of product gas composition versus oxygen flow rate

The effect of oxygen flow rate was studied on product gas composition. The compositions of H_2 decreases with very small deviation . The composition of CO and CO_2 increases with increase in the oxygen rate which means that in the stoichiometric reactor the reactions of carbon with oxygen i.e. complete and partial oxidation takes place.

VI. CONCLUSIONS

A simulation study using ASPEN PLUS was performed considering a coal sample using its proximate and ultimate analysis and the effect of various operating parameters was studied on the product gas composition.

Simulation trials were conducted by varying the steam flow rates thereby changing the steam to coal ratio whereas the coal flow rate and all other parameters were kept constant. A decreasing trend in the product gas composition of all the constituents was observed (Fig. 5) but the decreasing effect was much significant when comparatively higher values of steam were used. The extremely low composition of CO_2 can be attributed to the simplifications used in the simulation. There is a competition between the several gasification reactions to reach completion so it is very difficult to access the product gas composition as it also depends upon the operating parameters. The purpose of gasification dictates the presence or absence of a gasifying agent. ASPEN PLUS simulator provides a great deal of help in accessing the performance of a unit operation.

VII.   REFERENCES

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