Design and Simulation Model of a Gasifier for the Production of Syngas

By

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CERTIFICATE

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DEDICATION

I would dedicate my thesis to my beloved parents and my supervisor for their endless motivation and encouragement.

ACKNOWLEDGEMENT

I feel privileged to express my gratitude and feel indebted towards all those people who helped, inspired and encouraged me during my research work and in compiling the thesis report.

I would like to mention here my gratitude and special thanks to Sir Shahid Hussain Ansari, who trusted me and provide me with any opportunity to highlight key aspects of gasification. I would like to thank Engr Samiullah Khan and Mahesh Kumar for their guidance and support.

ABSTRACT

Production of syngas by gasification of locally available coal in the moving bed gasifier is one of the most economical and promising options to produce high calorific value gaseous fuel. Syngas contains significant amounts of C_1—C_4 hydrocarbons. Regarding the current situation of energy crisis and increase in the cost of conventional fuels (i.e. furnace oil) biomass and coal seems to be a cheap and accessible fuel in this part of the world. In these prevailing circumstances, syngas from surface mined coal gasification could be suitable alternate for limited natural gas. A moving bed gasifier designed by Aspentech in 2010 has been used to get some important results using local lignite coal samples, which are helpful in analyzing the potential of this conventional fuel. For this study, Aspen-Plus V8.0 has been utilized to simulate the performance of gasifier. The gasifier can withstand the temperature of 950°C and a pressure of 3.5MPa. Several numbers of RCSTRs are used to specify gasifier in the model, which utilizes 5 kg/s of coal after drying and pyrolysis. In this study steam is used as a gasifying medium. The R-yield reactor is used for pyrolysis in the modeling. Particle size distribution (PSD) is not considered in the model and coal feed is assumed to be pretreated to remove excessive moisture to 5 % in the proximate analysis for the simulation in gasifier. Fortran Subroutine codes built in the model were used for obtaining the mass and energy balances for the different process steps within the syngas production process. Sensitivity analysis and process optimization is done by considering pyrolysis temperature and S/C ratio as input variables. Based on this investigation, critical process steps for process heat integration and syngas yield are identified.

Keywords: Syngas, Particle Size Distribution, Pyrolysis, S/C Ratio, RCSTRs.

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Research Publication

1. “Optimization of Process Conditions for Production of High BTU Value Syngas by Simulation Model of a Moving Bed Gasifier” Bioenergy Conference 20-22 Nov, 2014 University of South Asia, Pakistan.

2. ** “Solid Waste Management & Integration with FTS Technology to Produce Syngas and Liquid Fuel” Bioenergy Conference 20-22 Nov, 2014 University of South Asia, Pakistan.

* Annexure I

**Annexure II

CHAPTER 1

INTRODUCTION

1.1 Background

Self-reliance in local energy resources is the reassurance for the country's economic development. In the light of recent fossil fuel consumption analysis, the most commonly explored oil and gas reserves will be exhausted in the subsequent half of this 21st century. Regarding the upcoming situation, to achieve self-sufficiency, substitute energy resources are being considered [1]. Conversion of solid coal into a gaseous fuel with high calorific value (or, hydrogen) is widely accomplished today. In the 20 to 40 years of the last century , coal gasification was a common practice to produce manufactured gas in number of plants around the whole world and such plants were generally known as manufactured gas plants (MGPs) in those times [2]. This technology lost appeal after World War II era because of the ample resource and supply of petroleum and natural gas at reasonable prices. However oil embargo enforced by gulf oil producing countries in the early 1970s and following increases and instabilities in petroleum prices, as well as the natural gas and petroleum shortage experienced during 2008-2009 when the whole world run into food and fuel crisis, the interest in coal gasification as well as its further commercial manipulation was invigorated [3].

Because of midterm exhaustion of oil and gas, coal gains significance not only as fuel providing cheap energy but also as feed for various industrial chemical syntheses. The available commercial gasification processes must be evaluated carefully for particular type coal feed to get best gasification yields [4]. The excessive ash, mineral and moisture content initially present in the coal feed are main challenges that arise in the coal gasification. The inclusive evaluation of gasification processes is challenging, as lots of governing variables such as coal structure and reactivity, temperature, pressure, steam requirement and other varying limiting conditions [2, 5].

1.2 Worldwide Coal Consumption and Production

Coal is the fastest-growing fuel in the last almost in every region of the world. Global production is greater than before by 6.1%. The Asia Pacific region is most prominent that is responsible for production growth of 85 % globally, led by china with 8.8 % increase the world’s leading consumer and supplier. Coal consumption increased by 5.4 % with Asia Pacific as the most prominent region in this net increase, while large regressions in North American consumption [6]. If production continues at this rate, world proven reserves of coal were abundant to meet hundred years of world annual production in 2011. Coal has the prevalent Reserve/Production ratio among other conventional fuels. Europe & Eurasia has the largest regional reserves and has the highest R/P ratio, which shows they were not completely exploited. Coal consumption grew by 5.4% in 2011, the only hydrocarbon fuel to exceed the average growth and the fastest-growing form of energy other than renewable. Coal had a share of 30.3% of global energy consumption, the highest since 1969. Global coal production has increased by 6.1% with non-OECD countries accounting for nearly all of the growth. China accounting for 69% of global growth [3, 6].

1.3 Role of Coal In Future Energy Mix Of Pakistan

The persistent energy gap in Pakistan can be reduced by the large local coal (lignite) resources at Thar in Sindh Province. This indigenous lignite coal can play significant role in Pakistan’s long term future energy security scheme [7]. The lignite resource has a worthy prospect to be a viable option for providing energy at low cost for long periods. Development of Thar is intended to begin with a corporation of government and the private sector, wherein the private sector would provide the necessary capital and make market profitable conditions and the government would provide the legal support, assisting to provide the necessary environment for such investments [8].

1.4 Thar Coal

Pakistan’s coal reserves were initially estimated to be about 186 billion tons of which 175 billion tones are present in Thar, Sindh (the largest lignite deposit in the world). Thar Coalfield is located in the eastern part of Sindh, 360 km from Karachi port in the southeastern zone. The coal rank is lignite B with an average heating value of 5,333 Btu/lb and sulfur content of 1.57 % and ash content of 8.83 percent. The dry and ash-free heating value for the lignite coals is 12,322 Btu/lb [9]. Thar Coal resources have been assessed for the potential of generating hundred GW of power for almost 300 years. Considering the abundant energy resource providing a commercial scale open cast mining & mouth mine power generation can be done over a long period [7].

1.4.1 Special Economic Zone

Sindh Thar Coalfield has been adjudged as a economic relieve zone and all Development Project in Thar region (including mining and power generation) have been acknowledged as, projects of national security [8]. Ever-increasing gas and oil prices in Pakistan severely affect electricity generation. IGCC plants were considered to have a advantage of being economically viable as compared to other conventional plants by using gas produced from indigenous lignite. Furthermore, catalytic coal gasification is technologically advanced as a more effective procedure to produce gasoline from coal [10]. Wood alcohol or synthetic gas can be produced from Thar coal at the qualified and can easily be transferred by pipeline throughout the country. The Shenhua Group of China has signed a contract with Sindh Government to investigate site and feasibility study for commissioning of 300MW coal-fired mine-mouth power plant established on their coal [8].

1.4.2 Future Buisness Potential In Thar Coal

Lignite Coal Resource located in the South Western Region Pakistan has a significant potential to play role in economic and energy sector. Coal recovered by open cast mining can be used in the local industries as cheap fuel providing energy mainly in cement and chemical processing plants. Synthesis gas produced from gasification can be further used to produce liquid hydrocarbon fuels like synthetic diesel.

1.4.3 Quality Of Thar Lignite

Thar lignite has stripped ratio of 6:1 and heating value ranging between 5,000 to 5,500 Btu/lb, depending on the moisture and mineral content which is better than most o th lignite coals found in different regions of the world being effectively used for mining and power generation [11]:

- Neyvelli lignite coal of India, which is being mined and operated by NLC has a strip ratio of 7:1 and heating value of 5,000 Btu/lb. More than 2,700 MW generations are based on Neyvelli lignite coal in India.
- Hungary’s lignite has a stripping ratio of 9:1 and a heating value 3030 Btu/lb and is used to generate electrical power, above 1800MW capacity.
- Rhineland Lignite of Germany has a strip ratio of 4.9:1 and heating value of 3800 Btu/lb and is producing power more than 10,200 MW capacity.

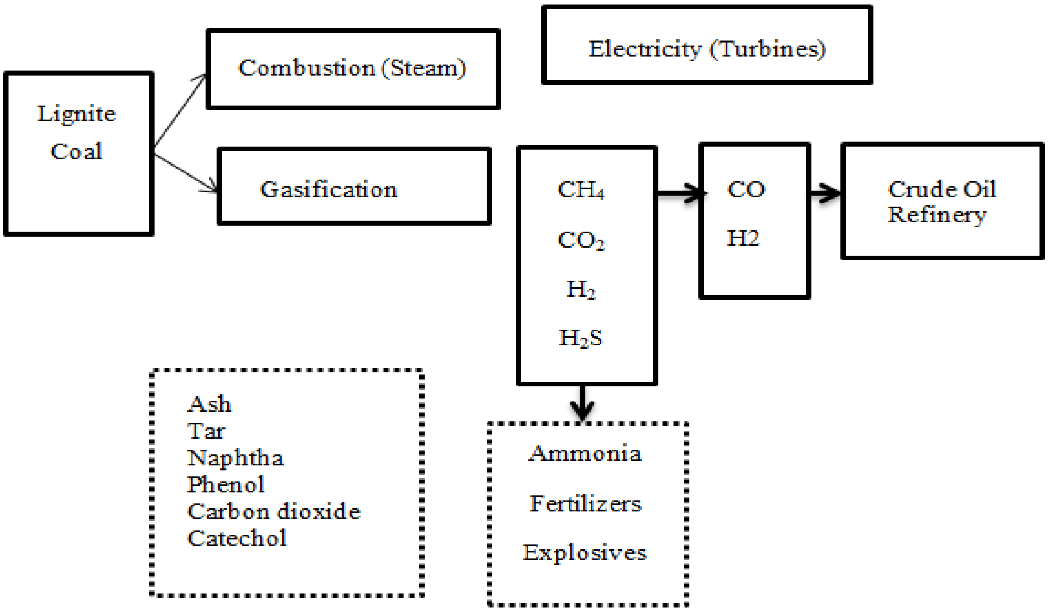


Figure 1.1 Petrochemical Products Obtained From Coal.

Table1.1 Worldwide Lignite Reserves With Respective Heating Values.

Deposit	**Stripping Rate (m^3: t)**	**Heating Value (MJ/kg)**
Thar Sindh, Pakistan	6.6 : 1	11.6
Rhenish Germany	4.9:1	8.9
Hungary	9 : 1	7.1
Greece	10:1	5.02
Kosovo	1:1	7.8
Hambach, Germany	6.8:1	10.5

1.4.4 Investment In Thar Coal Blocks

In the recent years, lots of efforts were made to develop infrastructure in Thar area to facilitate private investments. A road network to connect it with the western part of Sindh. Availability of telecommunication facilities and power lines near operational area of mine. Coal washing and environment monitoring units should be there. Railway lines to serve as source of transporting coal to other power plants. An Australian company has signed a memo with Sindh government. Feasibility study for underground coal gasification to produce syngas is complete. Commissioning of 1200 MW power plant in Thar Block-5.

Table 1.2 Thar Coal Field Investment Status.

Thar Coal Blocks	Status Timelines
BLOCK 1 Global Mining Company (GMC) Of China 900 MW generation from open cast mining Of 10 mtpa Coal feed supply to local thermal power plants	Bankable Feasibility Completed Planned Coal Production By 2015-2016 Power Generation Commencing By 2017-2018
BLOCK 2 Sindh Engro Coal Mining Co. (SECMC) (Shares in JV 51 % GoS, 49 % Engro) 600 MW generation from open cast mining of 6.5 mtpa	Bankable Feasibility completed 2010 Sovereign Guarantees by GOS for mining approved to facilitate by Chinese financial institutions Ground Breaking held 14 March, 2013 Over burden removal on Jan 2014 Project plans to reach 3.5 years 2017
BLOCK 5 Underground coal gasification Project And Power plant Planned	36 test bores have been drilled so far for coal seam analysis Test burn completed in Dec 2011 and syngas being analyzed. Power plant of 8-10 MW is being set up
BLOCK 6 Oracle Coal Fields PLC UK Open cast mine of 2.2 mtpa	Detailed feasibility completed April 2011, Start of mine development 2014 Agreement with KESC for 300 MW

1.5 Lurgi Gasification

Lurgi process was first acquired to produce town gas by thorough gasification of brown (low rank lignite and bituminous) coal in Europe. In late 1930s, the Lurgi gasifier process went operational for the first time on commercial scale. It initially raised one mmscf/d town gas utilizing lignite coal. Since 1966, there were number of Lurgi plants in Europe and Asia which were being operated to produce syngas [2].

Steam and oxygen are the two gasifying mediums used in almost all type of gasifier like Winkler, Lurgi and Koppers-Totzek process. Most of the advancements and improvements in gasification were observed in European countries. Of these all developments only few got attention and appreciation in U.S till 1970s, when oil embargo was imposed by Gulf countries. The other reason behind is discovery of natural gas as suitable gaseous fuel and also because of frequent and continuous supply of liquid petroleum products. After the oil restraint put up by Gulf countries in 1973,very serious vigorous and dynamic research and development efforts were steered for clean and efficient use of coal resources in coal gasification, coal liquefaction and IGCC [10]. Since, then most of the coal operating power plants have considerably improved their eminence of operation and working in terms of energy efficiency, by-products and emission control resulting in increased profitability [2].

1.5.1 Lurgi Dry Ash Gasifier

In dry ash gasifier, coal feed particle size is between 1.5-4 inch mesh screen that reacts easily with steam and oxygen in a moving bed. The process is operated in continuous mode. The gasifier is fortified with below mentioned hardware parts [2, 12]:

i. A coal lock chamber feeding coal from a coal storage bin in semi continuous mode to the pressurized reactor. This top metallic portion is frequently known as coal lock hopper.
ii. Coal distributor which rotates to distribute feed uniformly in the moving bed.
iii. A grate which revolves just below the combustion zone in gasifier from where steam and oxygen is introduced in reaction zone and the ash is removed from gasification and combustion zone.
iv. Ash lock chamber which discharges unreacted char and ash from pressurized reaction zone into an ash bin, ash is cooled by water quenching.
v. The hot product gases flows from gasifier to gas scrubber where heavy hydrocarbons are removed before syngas enters the waste heat boiler. The gasifier shell is installed with water jacket and cooling water flows inside it to control the temperature in gasifier. This water jacket also produces part of steam required for main process. An automated distributor is installed at the top of the moving bed, which uniformly spreads the feed coal [13].

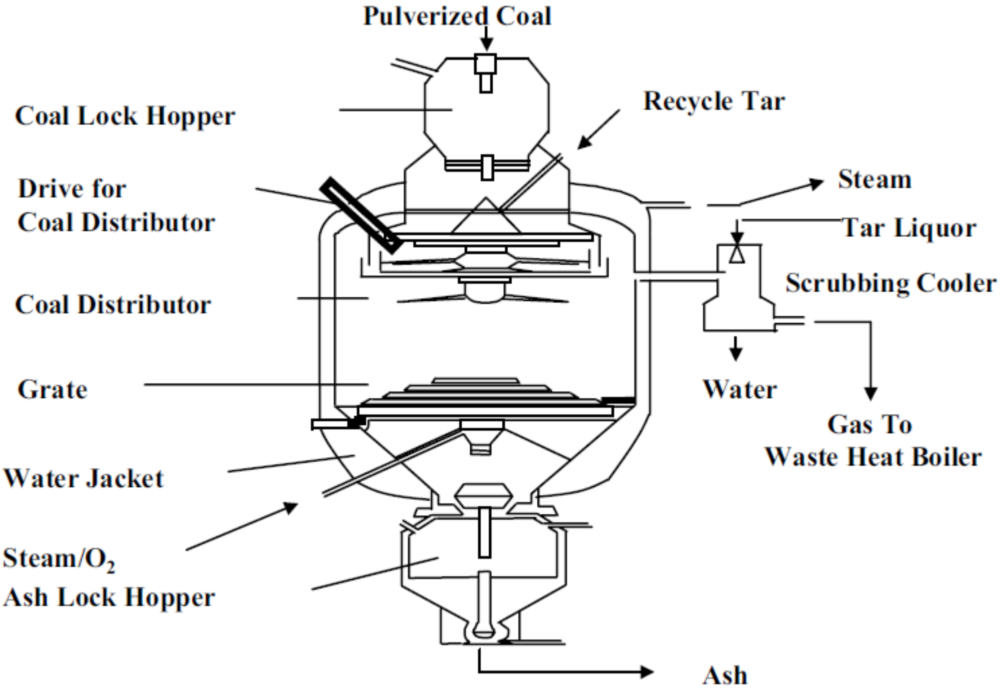


Figure 1.2 Lurgi Dry Ash Gasifier.

The grate just above the bottom of the reactor is also motor driven to remove unreacted char and ash into the ash lock hopper. There are several zones lying between the inlet and outlet grates. The zone at the top of gasifier preheats the solid coal and drying is done here by contact with the hot product gas that is released into the gas scrubber. Coal gets heated which facilitates in the removal of volatile components and pyrolysis is dominant in this zone proceeded by gasification reactions which occur at temperatures ranging between 620 to 760°C [14]. Gasification and combustion of char take place that is resulted in Devolatalization. The interface between pyrolysis and gasification is a significant defining factor in the reaction kinetics of char reactions, as well as the product gas composition and heat content. Combustion zone is at the bottom of the reactor, where the carbon in the coal reacts completely with oxygen to yield mainly carbon dioxide [15]. The heat produced in combustion reaction is consumed by gasification and pyrolysis zone reactions which are endothermic reactions. Energy assimilation is accomplished in gasifier by utilizing the heat of combustion in the gasification and pyrolysis, both of which require heat to proceed [16]. Almost 20% of feed coal is burnt completely while the rest is gasified. The percentage burned coal feed for heat utilization purpose may be termed as sacrificial coal. The combustion zone temperature must be set lower than an ash fusion point, but should be high enough to influence gasification and combustion effectively in their respective zones [2]. This temperature is also adjusted by steam to oxygen ratio. The stoichiometric balances of material and energy in Lurgi gasifier is evaluated by limiting following process variables [2, 15]:

i. Gasifying temperature, pressure and O/C, S/C mass ratio.
ii. The rank and nature of coal define the extent of gasification and pyrolysis reaction. Lignite is the most reactive among other types of coal, gasification reaction proceeds at 650C for this low rank coal. Contrary to this, coke and anthracite are least in reactivity, for a chemical reaction to occur minimum temperature is kept near 840 C. Thus, mass of coal gasified unit mole of gasifying medium (oxygen) for lignite matched to bituminous and sub-bituminous coal. On the scale reactivity of coal decreases as rank of coal moves upward (i.e., the carbon content of coal).
iii. The ash fusion point of the coal and steam, oxygen flow rates determines the maximum operable temperature in a dry ash gasifier.
iv. Lurgi gasifier has a high thermal efficiency compared to batch gasifier because of its moderate pressure operation and the counter current flow of solid-gas interaction. The Chemical composition and amount of volatile matter present in the coal has the significant impact on quality and measure of heavy hydrocarbon formed and tar. Nevertheless, it needs high flow rates of steam and the large amount of carbon dioxide is produced in product gas and syngas temperature coming out of gasifier is at high temperature. Likewise, the crude syngas leaving the gasifier which constitutes oil, naphtha and tar which are removed in subsequent treatment blocks. These carbonization products are formed in pyrolysis zone and reactions in which intermediates are formed. This crude syngas is subjected to post treatment in gas scrubber and waste heat boiler moving downstream [2, 14].

1.5.2 Slagging Lurgi Gasifier

Slagging Lurgi gasifier is an improved and upgraded version of dry ash gasifier. The temperature of the combustion zone is higher than the ash fusion point to gasify almost 90 % of the coal feed. The above mentioned objective is accomplished by suppressing the flow rate of steam than dry ash Lurgi gasifier, consequently depressing the steam to oxygen ratio. The ash removed as slag is collected at the bottom, not in dry form. Henceforth, the process is effective for coals capable of forming cake; unlike the former dry ash gasifier. The main advantage of this gasifier is more quantity of carbon monoxide and hydrogen in syngas, yielding syngas of high heat content. The coal material conversion is increased significantly. The steam required for gasification is also reduced [2, 13].

1.6 General Aspects Of Gasification

For all the gasification reactions that takes place, the conversion and reaction rate kinetics are typical functions of gas composition, nature and rank of coal, mineral content and moisture content of coal and operating variables like temperature and pressure. For a specific type of gasification reaction the equilibrium of reaction shifts by either decreasing or increasing the temperature in all types of gasifier [13]. In general, the rate of reaction increases with small increase in temperature. However, in some particular reactions, the effect of pressure change cannot be ignored; it also effects the product gas formation [12, 17]. Thermodynamics of carbon and hydrogen gasification reactions shows that methane production is enhanced at high pressures like 50 to70atm and temperatures ranging between (760-930C). In case of syngas production, at low pressure and high temperature yield is maximum (i-e, carbon monoxide and hydrogen) [14, 18]. Heat provision and heat recovery is an important element in gasification from the viewpoint of cost, design specification and operability. Char formed in pyrolysis is oxidized partially with steam leading to generation of heat and synthesis gas. The reduction and oxidation of iron ore in the cyclic manner is another way to produce a synthesis gas stream associated with heat [2, 13]. Downstream operations and further treatment of syngas depends on the rank of coal initially used in gasification. An Entrained flow gasifier on the hand is capable of handling almost any quality of coal feed, because the feed injection mechanism is different, forming a slurry or suspension of feed. However, if caking coals were gasified in a fixed bed or fluidized bed, some important changes are done and special methods are employed to prevent caking. If cake formation or agglomeration happens in gasifier it seriously effects the normal operation of gasifier in long runs [2].

Gas leaving contains sulfur in the form of sulfur dioxide, hydrogen disulfide or mercaptants, depending upon conditions and the nature of the reaction. Sulfur dioxide is produced if the oxidizing environment is there in the operation of gasification. The volatile matter (VM), fixed carbon content (FC), and the moisture content also plays an important part in coal treatment needs and processing in gasification [13, 16]. The sulfur and nitrogen contents of coal determine whether post treatment and waste heat removal requirements are significant. Sulfur may exist in three different types in coal, namely pyritic sulfur, organic sulfur and Sulfatic sulfur. The first two mentioned are more frequently found in coal whereas the last one is present in oxidized or wind swept then fresh coals [2].

1.7 Objectives Of Current Study

Simulate a moving bed gasifier model using local coal. Using bore-hole data obtained from initial drills including proximate and ultimate analysis of lignite.

Specifically focused on:

- Effect of pyrolysis temperature on syngas composition.
- Effect of steam flow rate on syngas composition.
- Carbon conversion through gasification and combustion zone.
- Top to bottom profile of H_2, CO, CH_4 and CO_2.
- Top to bottom profile of solid carbon and sulfur.

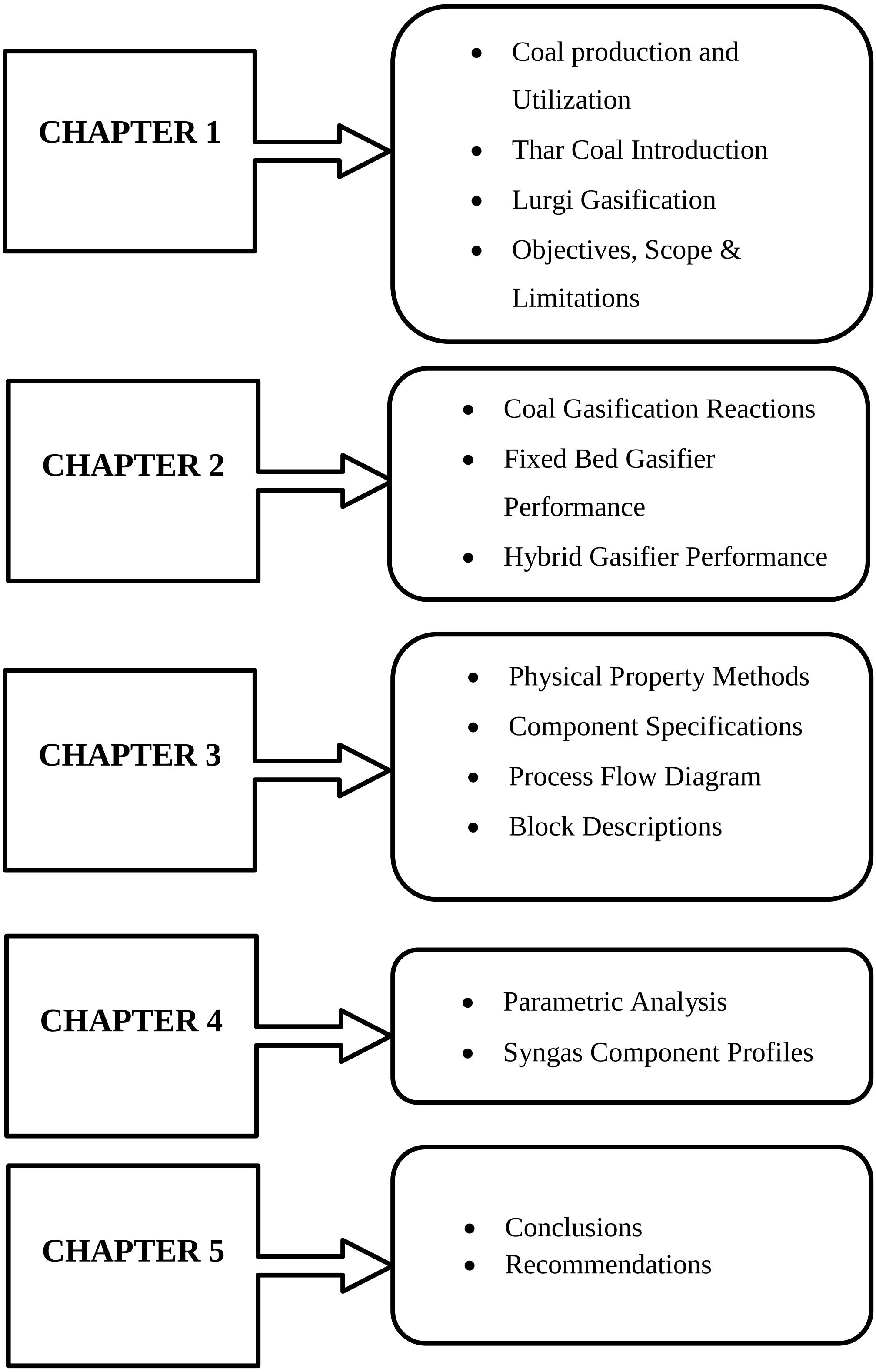
1.8 Limitations And Scope

Countercurrent moving bed gasifier is used for parametric analysis of bituminous and lignite coal. Individual component profile of syngas component, solids and temperature were observed throughout the gasification and combustion zone. Pyrolysis product from bituminous coal and lignite are compared.

Coal feed is considered to be initially pretreated to remove excessive moisture. Coal particle size is 0.02 m with considering no PSD in the model. Steam and oxygen being used as utility are not produced, but flow rates are specified. Pressure drop in gasifier is not taken into account in the simulation.

1.9 Organization of Thesis

Thesis comprises of following chapters. The detail of chapters is mentioned in the flow chart below:



Summary

The current situation of Pakistan in terms of energy unavailability and a large share of oil and gas in the overall energy mix leads to the future problem of energy security. The gas reserves will be soon exhausted if continued at same consumption rate. The huge amounts of furnace oil imported for power generation also affects the economy of the country. Utilization of indigenous energy resource especially coal is the best solution for getting cheaper energy. Some serious efforts and initiatives were taken by the Government of Pakistan and the private sector to develop this local energy resource. Worldwide coal consumption and production is discussed in detail. Thar coal field financial investments and future developments are enlisted. Lurgi Gasification process along with its types and operating principle are discussed. Objectives of study and limitations are mentioned at the end.

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CHAPTER 2

LITERATURE REVIEW

2.1 Coal Gasification Reactions

In almost all types of gasifiers, with different symmetry and principle, following major reactions occur simultaneously [1]. The equilibrium constants of these reactions are shown on table below as function of gasifier operating temperature. The graphical representation is shown in figure. Following significant conclusions are drawn from the figure [2]:

i. The curve between $\log_{10}K_p$ and 1/T is almost linear for all the reactions.

ii. The amount of heat necessary for the reaction to proceed (exothermic reaction) is equal to the slope of the curve $\log_{10}K_p$ and 1/T for individual reaction curve.

iii. At low temperature, hydrogasification is preferred thermodynamically for which criteria is $\log_{10}K_p>0$. On the contrary to this carbon dioxide and steam gasification reactions takes place at high temperature.

iv. For WGS reaction, equilibrium constant shows significant variation with temperature change as compared to all other chemical reactions that shows little or negligible variation, which is clear from the figure. Equilibrium of WGS reaction can be easily shifted by changing operating parameters as compared with all other reactions in the process [3].

2.1.1 Steam Gasification

The heat input is essential for steam gasification reaction to proceed due to its endothermic nature.to enhance the rate of reaction in limited time steam is supplied in excess [4]. The carbon and gaseous reactants mechanistic chemistry is being discussed here precisely, but not for reactions that occur between gaseous reactants and solid carbon. Carbon has the maximum percentage value in coal as it is clear from the proximate analysis of lignite coal. But, the reactivity of carbon is different from other elements and compounds present in coal. In normal practice pure carbon is less reactive as compared to coal because there are number of various reactive compounds present in the coal which alters it overall reactivity and they also play role as catalyst in many chemical reactions, altering the rate of reaction [1]. Mineral matter present also increases the reactivity of coal depending on the nature of minerals present. Anthracite has the highest percentage of carbon in proximate analysis and is best in rank among all types of coal but offers least reactivity and is most unlikely and difficult to gasify or liquefy because it requires lots of heat and elevated temperatures to gasify this solid fuel. The carbon deposition reaction occurs at good rate when steam supplied in gasifier is low [5].

Table 2.1 $Log_{10}K_p$ Values for all Gasification Reactions.

T (K)	1/T (1/K)	$Log_{10}K_p$					
		I	II	III	IV	V	VI
300	0.00333	23.93	68.67	15.86	20.81	4.95	8.82
400	0.0025	19.13	51.54	10.11	13.28	3.17	5.49
500	0.002	16.26	41.26	6.63	8.74	2.11	3.43
600	0.00166	14.34	34.4	4.29	5.72	1.43	2
700	0.00142	12.96	29.5	2.62	3.58	0.96	0.95
800	0.00125	11.93	25.83	1.36	1.97	0.61	0.15
900	0.0011	11.13	22.97	0.37	0.71	0.34	0.49
1000	0.001	10.48	20.68	0.42	0.28	0.14	1.01
1100	0.00090	9.94	18.8	1.06	1.08	0.02	1.43
1200	0.00083	9.5	17.24	1.6	1.76	0.16	1.79
1300	0.00076	9.12	15.92	2.06	2.32	0.26	2.1
1400	0.00071	8.79	14.78	2.44	2.8	0.36	2.36

Where, Reaction no are shown in 2.1.2

2.1.2 Carbon Dioxide Gasification

The reaction between carbon and carbon dioxide produced in combustion reaction is known as boudouard reaction. This reaction is of endothermic nature and requires heat to proceed similar to the steam gasification reaction[2].

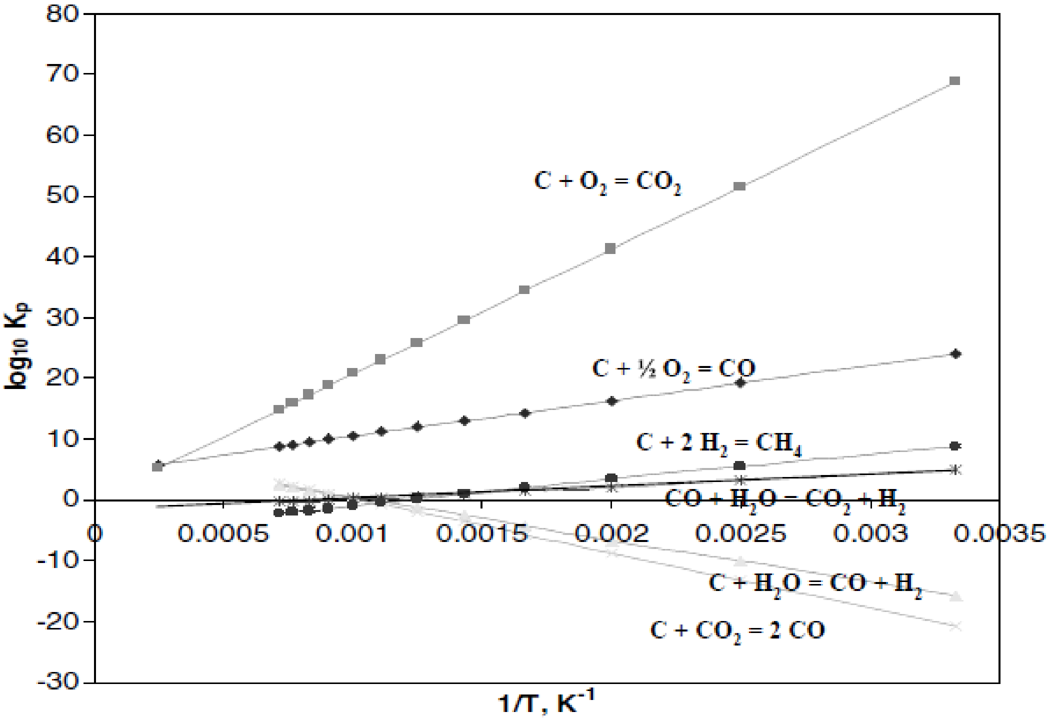

Figure 2.1 Plot Between 1/ T and $\log_{10}K_{p}$.

For reaction to occur separately it requires very high temperature and pressure (for reaction rate to be satisfactory). When reactant concentrations are higher than normal high pressure is required to get maximum conversion [2, 3]. The boudouard reaction is difficult to be carried out separately as it is not cost effective; highly energy intensive, slow reaction rate problem and minimum conversion are the major problems that practically arise. Methane can also be produce by addition of hydrogen gas to the lignite coal at very high operating pressures. The reaction is commonly termed as hydro gasification [6].

$$H_2 + 0.5O_2 \rightarrow H_2O \qquad (2.1)$$

The reaction mentioned above generates heat, in that it is preferred at low operating temperatures because of the exothermic nature. The temperature preferred for reaction is below 670°C, which is opposite to the steam and carbon dioxide gasification reactions [7]. At low to moderate temperatures the other problem that arises is slow reaction rate. Thus, for reaction rates being high and better kinetics of process temperature is kept on the higher side. For syngas production, high pressure shifts the equilibrium in syngas formation. The overall cost and economics of process increase with the use of catalyst, making difficult to justify the process on economic grounds because the exhausted catalyst recovery posse a serious problem and its recycling also requires energy and cost for the removal of unreacted char and ash and regeneration [1]. Consequently, the above mentioned complications are the main reasons due to which catalytic gasification is not practiced widely on commercial scale [8].

2.1.3 Partial Oxidation

Coal combustion reaction with oxygen, which can be provided as pure or as fraction of air results in carbon monoxide and carbon dioxide.Major reactions occurring are shown below: Principal chemical reactions between carbon and oxygen involve [6]:

$$C+\frac{Z+2}{2Z+2}O_2 \rightarrow \frac{Z}{Z+1}CO+\frac{1}{Z+1}CO_2 \tag{2.2}$$

If the amount of air or oxygen supplied is just sufficient or stiochiometrically required, then vapour- phase oxidation and ignition of volatile matter is the phenomena by which combustion proceeds sequentially and eventually leading towards the ignition of residual char. To continue combustion reaction for a long time results in the inadequate use of carbonaceous solid, that’s why it is not desirable. Although the expressions for combustion and oxidation reactions are simple equation, but the partial oxidation mechanism is complex and which depends on how quickly and efficiently combustion reaction proceeds [9]. Due to the presence of both heterogeneous and homogeneous reactions the pathway of the main reaction is further complicated to understand. The inital The early argument hat arise in carbon oxidation reaction is whether in heterogeneous reaction of oxygen and carbon the main product is carbon dioxide or the other suppressed product is carbon monoxide in gas phase oxidation reaction [3].

2.1.4 Water Gas Shift (WGS) Reaction

WGS reaction is not the prime centered reaction in gasification reactions, yet its importance in chemical reaction systems and synthesis gas is very much significant. The equilibrium for WGS reaction is least sensitive among all other reactions when temperature variation is considered [2, 3]. It can be concluded with other words that its equilibrium constant has almost no effect of temperature change. Thus, equilibrium for WGS reaction does not shift for long range of temperature variation in operation. WGS reaction when proceeds in the forward direction is slightly of exothermic nature [2]:

$$CO + H_2O \leftrightarrow CO_2 + H_2 \tag{2.3}$$

Scientists and chemist still have believe that reaction takes place at the coal particle surface and is of heterogeneous type and is catalyzed by solid carbon surface. However, on the other hand all the chemical species participating in the reaction are in gaseous state. It is difficult to understand and develop a generalized approach regarding WGS reaction as it is being catalyzed on heterogeneous surfaces, also the reaction is homogeneous and heterogeneous in a sense as mentioned above [1]. For commercial scale reactor, the rate kinetics information available in the literature is not of much use and worth. Methanol production from syngas can be achieved by keeping the hydrogen and carbon mono oxide ratio 2:1 and operating the gasifier at low pressure specially in vapor phase [8]. Balanced gas is term used for consistent syngas produced from above methodology on the other hand syngas composition that differs from basic principle reactions is known as unbalanced syngas [6]. If high yield of hydrogen is required in syngas then hydrogen to carbon monoxide ratio should be further increased by mainly GS reaction and converting mostly produced CO into carbon monoxide. If the hydrogen produced by syngas mixture is to be used in fuel cell applications, carbon monoxide and carbon dioxide should be removed to the minimum level by adsorption process or either employing acid gas removal unit [3].

2.2 Lurgi Fixed Bed Gasifier Performance

Aspen plus simulator is being used to develop a commercial scale model of pressurized Lurgi gasifier which in itself is a steady state kinetic model. The model developed is used to investigate thermodynamic efficiencies, individual component profiles of throughout the whole gasification system and were studied in detail [4]. Five important zones, namely; drying, pyrolysis, gasification, combustion and overall heat recovery blocks were used to illustrate these zones individually. A mathematical model which is stoichiometric ally evaluated and an external FORTRAN language subroutine code that apprehends syngas composition produced in Lurgi gasifier is encoded and integrated with the model [7]. The difference between industrial data and the model simulated value is very small and is in good agreement. The model is developed to analyze the effect of steam to coal mass ratio and oxygen to coal mass ratio on the thermodynamic efficiencies of the gasifier and the complete system that is being used for gasification [6]. The exergetic efficiency for the combustion zone in the Lurgi gasifier has serious impact and change observed when oxygen in the coal mass ratio is varied. On the contrary, to those for gasification the exergetic efficiency shows no appreciable change and is almost insensitive to the change in oxygen to coal mass ratio. The results observed for steam to coal mass ratio are opposite to the above mentioned case. For gasification the exegetic efficiency is much variant to change in steam to coal mass ratio when compared with combustion zone. The maximum value of 72 % of exergetic efficiency is achieved for the steam to coal mass ratio of 0.85 and oxygen to coal mass ratio of 0.19 [6].

2.2.1 Model Validation

The validation of Lurgi gasifier model with industrial running data, makes it a good tool to analyze the mainly the performance of gasifiers by studying the effects of steam and oxygen to coal mass ratio.all the variables in the model were the same values as in Run 1 except the change in steam to coal mass ratio and oxygen to coal mass ratio. The operating temperature inside the gasifier and carbon conversion rates are determined by the important parameter oxygen to coal mass ratio. The above mentioned effect in a gasification system of Lurgi gasifier is illustrated graphically figure 2.2:

2.1.1 Syngas Ratio

The important and significant factor involved in petroleum and petrochemical production through FT synthesis is syngas ratio. The syngas ratio of the product gas obtained from the combined gasification process is being investigated. It is observed that with the increase in the temperature syngas ratio decrease [10]. The temperature in this study is varied from 500 to 1200° C at constant remain in gasification variables. It was also analyzed in the study that increase in feed carbon monoxide moles results in decrease in syngas ratio and this is investigated at constant temperature for all cases [10].

To observe and analyze the effect of pressure, temperature and carbon monoxide feed along with the steam flow rate of synthesis gas composition a thorough study of lignite coal gasification considering the thermodynamics of the process [4]. The syngas ratio and enthalpy of product gas is also determined for any change. Carbon dioxide produced in excess during gasification and combustion reactions is essentially consumed in the combined gasification process which also results in reduced carbon footprints in the whole process. The use of oxygen rather than air for gasification yields more valuable components in final synthesis gas, because excess nitrogen is not there which would have accompanied if air is used as gasifying medium [6]. The steam consumption in the pure steam process is much high as compared to the combined gasification process while it also facilitates the carbon dioxide gasification reaction which requires steam. The uses and quality of syngas were also studied. For production of valuable products through the FT synthesis of syngas, syngas ratio must be kept low in the range between 1-3 [11]. For synthetic natural gas syngas ratio is also kept on the lower side. The syngas is suitable for applications in fuel cells if nitrogen is not present in the final product. In combined gasification external energy is required to carry out the process and achieve maximum conversion. But in some cases carbon conversion could be achieved at low temperature and syngas produced does not have large nitrogen fractions, thermo neutral gasification operation in combined gasification [3].

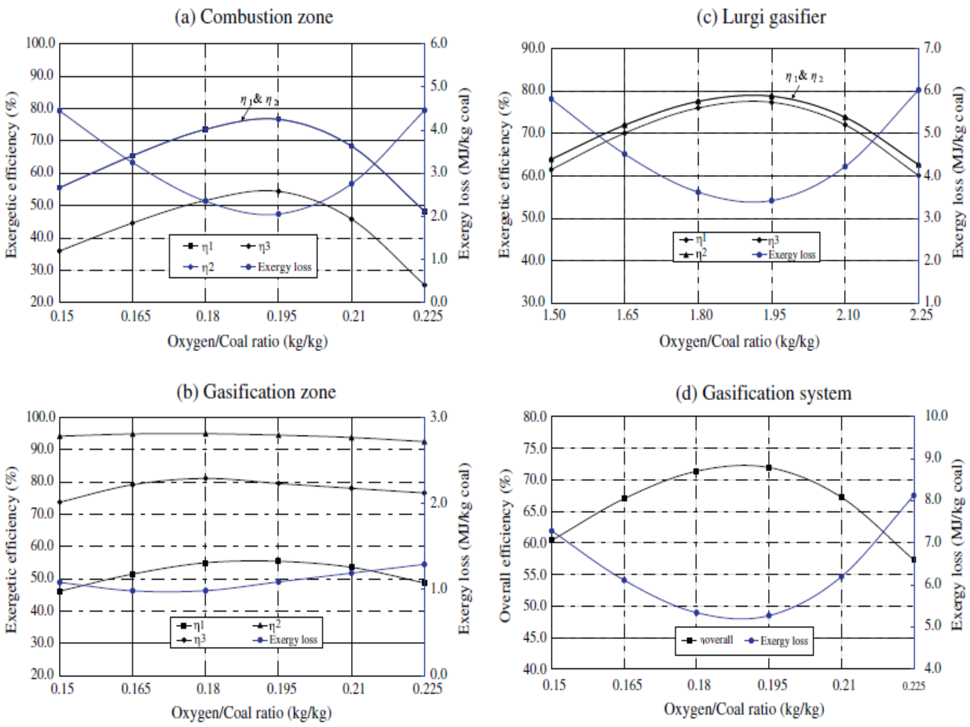

Figure 2.2 Exergetic Efficiency in gasification and combustion zone

2.2 Hybrid Gasifier Model

Aspen simulator is being used to develop a steady state model for hybrid gasifier utilizing biomass for gasification. The model results were validated by comparing with la scale hybrid gasifier. The variable operating parameters were considered in the model for parametric analysis for analyzing the gasifier performance and the results were close to practical values obtained from lab scale gasifier [10]. Parametric analysis was done and the effects of changing equalance ratio, operating gasifier temperature, moisture content in carbonaceous biomass were observed on th syngas final composition. Higher heating value of syngas and hydrogen production in syngas were also investigated for each case. It’s usually concluded that at higher temperatures gasifier performance is better. This is attributed to the production of carbon monoxide and hydrogen, which finally produces syngas having high heating value. Equivalence ratio has a direct effect on carbon conversion and the reaction kinetics of almost all the reactions involved in gasification process [10]. High moisture content in the initial feed biomass decreases the overall performance of the gasifier and results in low heating value gas. By increasing the steam flow rate supplied in the gasifier hydrogen yield is maximized but he heat input to the chamber also increases so an optimum steam supply is needed to avoid excessive heat loss.

Among the three types of biomass waste considered in the model food waste shows highest carbon monoxide and hydrogen yield in syngas and HHV of 71 %. For other two biomass feeds namely poultry and municipal waste syngas quality is satisfactory and can be improved by enhanced mixing inside the gasifier [12].

2.3 Downdraft Fixed Bed Gasifier

Gasification performance of downdraft gasifier is being analyzed which utilizes torrified and raw bamboo as feed for gasification. The model is being developed using Aspen plus simulator for fixed bed down draft gasifier. It was observed that by keeping torrification temperature, high the syngas yield can be appreciably increased both in quality and quantity. Yet, the TB has much higher heating value as compared to its counterpart raw bamboo [10]. By decreasing the modified equivalence ratio and increasing steam flow rate ratio, Carbon monoxide and hydrogen production is maximized for the raw bamboo gasification scheme. The overall impact of above mentioned change is an increase in carbon conversion and efficiency. In case of syngas production terrified bamboo is efficiently gasified higher steam flow rates, because the carbon content in biomass fuel is high. Carbon conversion is lower for torrified bamboo because of its higher carbon content as compared to other types bamboo used in gasifier as fuel. Torrified biomass 250 is most appropriate and suitable fuel to be gasified when syngas composition and yield, carbon conversion are simultaneously considered. The torrification of biomass requires a set of extra equipment to carry out operations and increase the overall cost of gasification. The energy requirements terrified biomass cooling and tar removal is required. In this study only TB250 and TB300 are used as biomass feed because of the scarce experimental and practical data available in this regard. Further evaluation and understanding of operating fixed cost requirements of torrification is needed to optimize the gasification which is dependent on it in economic terms. The process could then be easily optimized [10, 12].

Summary

Coal gasification reaction mechanism from different studies is being discussed in detail. Performance analysis of Lurgi fixed bed gasifier is discussed with the effect of steam to coal mass ratio and oxygen to coal mass ratio on syngas composition. Exergetic efficiency optimization regarding S/C mass ratio and the O/C mass ratio was observed. Model results validation with industrial data and the effect of syngas ratio is mentioned. Aspen simulator use in developing different models and their specification is enlisted above.

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CHAPTER 3

METHODOLOGY

3.1 Background

Moving bed coal gasifier is a vertical reactor. Coal feed reacts with gasifying medium to produce the gas containing CO, H_2, CO_2, CH_4, and other hydrocarbons. Coal is fed into the hopper at the top of the gasifier and moves downward due to gravity. Oxygen and steam are introduced at the bottom of the pressurized gasifier. Four processes that take place in sequence from top to bottom: coal drying, coal pyrolysis, char gasification, and char combustion [1].

Ash and unreacted char are removed by the rotating grate at the bottom, and the product syngas leaves at the top. Part of steam used in gasification chamber is produced by a water jacket surrounding the chamber [2].

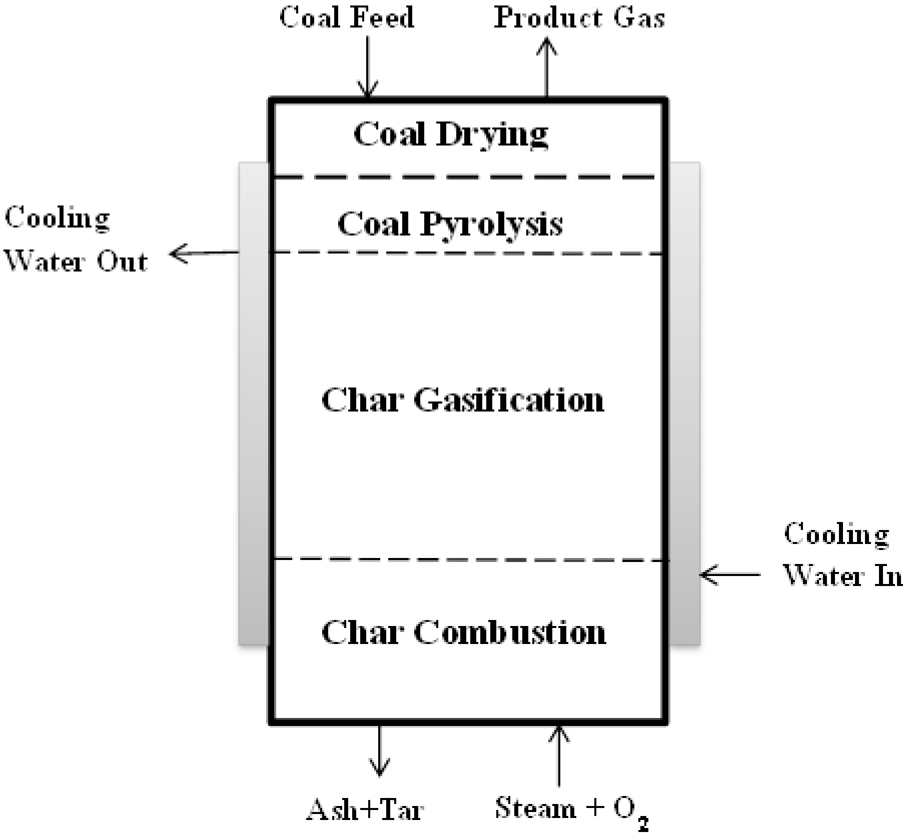

Figure 3.1 Moving Bed Gasifier.

3.2 Physical Property Methods

The property method RK-SOAVE is used to evaluate the physical properties of MIXED conventional components and CISOLID components. HCOALGEN and DCOALIGT models are selected for enthalpy and density calculation of non-conventional components, respectively [3].

3.2.1 Rk-Soave Equation

$$p = \frac{RT}{v_m - b} - \frac{a}{v_m(v_m + b)} \tag{3.1}$$

Where, P is the gas pressure R is the gas constant, T is temperature, V_m is the molar volume (V/n), a and b are constants that corrects for attractive potential of molecules and volume. The details of a and b constants can be obtained from literature [4, 5].

3.2.2 HCOALGEN

The HCOALGEN model for enthalpy calculation requires these component attributes for non-conventional components:

- Proximate analysis results (PROXANAL in Aspen Plus)
- Ultimate analysis results (ULTANAL in Aspen Plus)
- Sulfur analysis results (SULFANAL in Aspen Plus)

Proximate analysis gives the weight content of fixed carbon, volatile matter, moisture and ash. The ultimate analysis gives the weight composition of coal in terms of ash, carbon, hydrogen, nitrogen, chlorine, sulfur, and oxygen. The sulfur analysis divides the sulfur content into three types, pyritic, sulfate, and organic sulfur [1, 3].

3.2.3 DCOALIGT

The DCOALIGT model for density calculation requires two component attributes ULTANAL and SULFANAL.

For the characterization of the char and ash generated in gasification of coal same methodology is applied as mentioned above and the same models are employed to evaluate enthalpy and density.

The results of proximate, ultimate, and sulfur analysis for the char and ash are determined from the analysis data of local coal and the amount of gaseous product in terms of mass balance.

3.3 Stream Class

The stream class used is MIXCINC with MIXED, CISOLIDS and NC sub streams. The coal feed temperature, pressure; flow rate and component attributes are specified in NC sub stream sheet. The model includes two material and heat streams, as shown in Block Diagram. The streams with solid lines represent material streams. The streams with dashed lines represent heat streams.

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3.4 Component Specifications

Components specified in the model were taken from component databanks Pure27, AQUEOUS, SOLIDS and INORGANIC .The molecular structure of components is being used as defined in Aspen plus.C_6H_6 was used define tar produced in pyrolysis block which also represents the amount of higher hydrocarbons [6]. Coal gas is composed of components lighter than C_6, including CO, H_2, H_2O, CH_4, CO_2 and C_nH_m ($n \leq 6$) [7]. The high-weight hydrocarbons, including tar, phenol, naphtha and oil, whose molecular weights are larger than that of C_6 are referred to as distillable organic liquids. The high molecular weight hydrocarbons produced during gasification and combustion of char have very small compositions and possess properties that of liquid at ambient conditions [2].

3.4.1 Component Attributes Of Thar Coal

Component attributes of Thar lignite were retrieved from modeling of bore-hole data, including proximate, ultimate and sulfur analysis which is shown in the table 3.1 [8]:

Table 3.1Analysis of Lignite Thar Coal.

Proximate Analysis		**Ultimate Analysis**		**Sulfur Analysis**	
Element	Value (wt. %)	Element	Value (wt. %) Dry Basis	Element	Value (wt. %) Dry Basis
Moisture (Wet Basis)	5.0	C	67.6	Pyritic	0.76
Fixed Carbon	37.33	H	5.6	Sulfatic	o.76
Volatile Matter	47.82	N	0.91	Organic	0.76
Ash	14.85	Cl	0	NA	
		S	2.28		
		O	16.4		
		Ash	7.21		
Calorific Value(GCV)		11.6 MJ/kg			

3.5 Process Flow Diagram

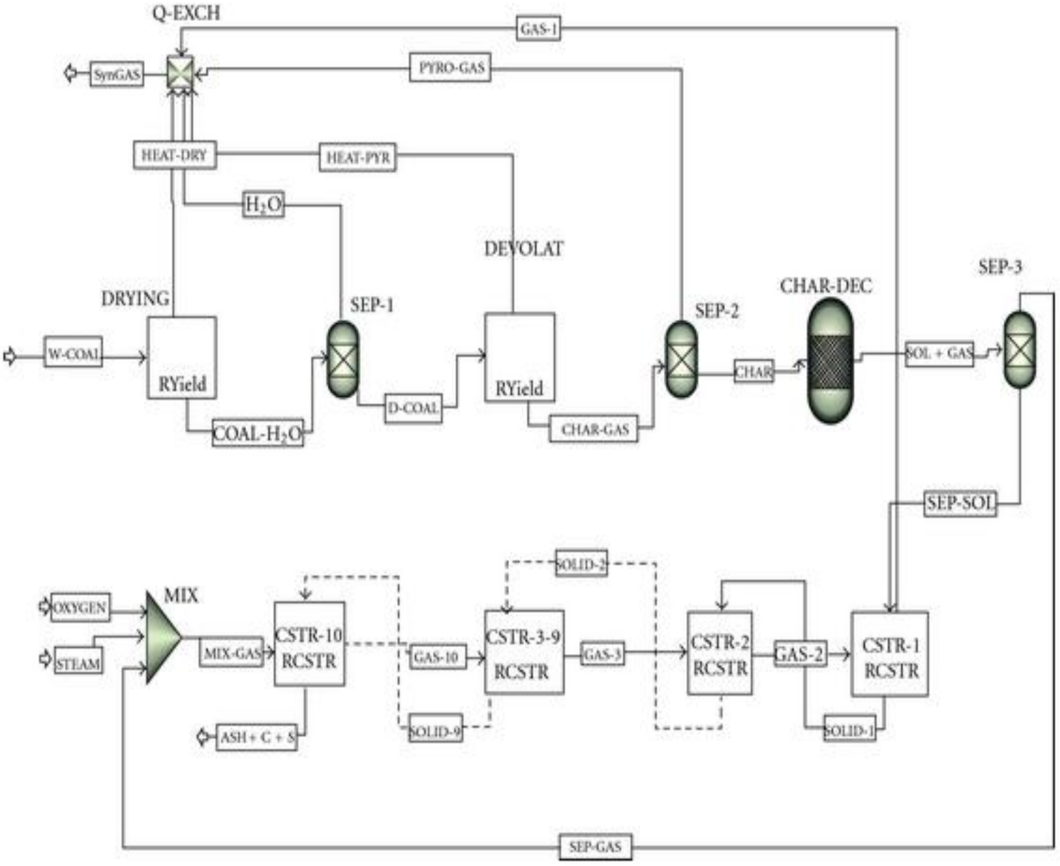

Figure 3.2 Process Flow diagram of Gasifier Blocks

3.6 Block Description

3.6.1 Coal Drying

The physical moisture bound in the coal particles, adsorbed on the surface or trapped inside the solid particles is released into the gas phase. Drying is being specified in the model by R-yield block. The yield of water vaporized is determined by initial moisture in the coal feed. For lignite coal, the water content is 5.0 wt. %, the mass yield of water vapors in drying block is 5.0%, assuming that physical bound water is completely removed from coal. The dried coal mass yield after removal of moisture is equal to 95 wt. % [1].

After drying, water vapors and dried coal enters into a gas-solid separator, SEP-1. The separated vapors are mixed with gas stream from coal pyrolysis, char gasification, and char combustion to produce the final syngas. DRY-COAL goes into pyrolysis block. In the process flow diagram, there is a heat stream Q-DRYING which represents the heat duty in the drying process. This stream is used to keep the heat balance inside the gasifier. The heat needed in the drying process is provided by the hot gases from coal pyrolysis, char gasification, and char combustion. The dried coal is represented by DRY-COAL sub stream in the model [1, 7].

3.6.2 Coal Pyrolysis

Pyrolysis step is of significant importance in the moving bed gasification. The coal pyrolysis phenomenon is still difficult to describe completely. It is difficult to relate the reaction kinetics to fuel properties/composition and such operating variables as particle size, constituents of carrier gas, temperature, pressure, residence time as well as heating rate. The fundamental thermodynamic/dynamic data are rather limited and hard to obtain[7]. There are two methods to estimate the range of each coal pyrolysis product. One is based on experiments (coal pyrolysis experiment outside the gasifier). The second one is a theoretical method using a functional group model. Due to the complexity of coal in composition, the theoretical method is very complicated and difficult to use in practical application [1].

The method based on experiments is most practical and preferred in simulation. So, the experimental method is used to predict the results of coal pyrolysis products. The dried coal is broken into CO, H_2, CO_2, H_2O, H_2S, N_2, CH_4, C_6H_6, and char. The yield of each component is specified according to the experimental results. The heat required in the pyrolysis process originates from the heat exchange with the gas from char gasification and combustion, represented by the heat stream Q-PYROLYS. After the pyrolysis, product flow into the gas-solid separator block (SEP-2). The gases from SEP-2 flow upward into the coal drying process. The solid char from SEP-2 flows downward into the char gasification and combustion processes.

$$\mathrm{Coal} \rightarrow \mathrm{CO} + \mathrm{H_2} + \mathrm{CO_2} + \mathrm{H_2S} + \mathrm{N_2} + \mathrm{CH_4} + \mathrm{C_6H_6} + \mathrm{Char} \quad \cdots\cdots\cdots\cdots\cdots\cdots \quad \text{(I)}$$

3.6.3 Char Gasification and Combustion

Coal drying and pyrolysis are assumed to happen instantaneously where coal is fed to gasifier at the top. The length for char gasification and combustion is equal to the total length of gasifier in the model as length of drying and pyrolysis zone is almost negligible. The moving bed coal gasifier is a counter current reactor, which indicates that to simulate the char gasification and combustion processes in countercurrent reactor model is required. Aspen Plus does not have a built-in reactor model to deal with the counter current reactor. Benjamin et al. developed a user solution program for the countercurrent moving bed coal gasifier, and then integrated it into Aspen Plus, but the solution was time consuming. This is attributed to the following reason:

The mathematical model of the countercurrent moving bed coal gasifier comprising of a single block is a two-point boundary value problem. Its solution requires matching a number of variables, some specified at the top and others at the bottom of the gasifier. This feature causes the solution process to be usually complicated. Directly using the built-in algorithm in Aspen Plus and simplifying the problem, a number of RCSTR reactors in series were used to model the char gasification and combustion processes. The RCSTR reactor has unique characteristic that gas and solid phases have the same temperature, which means temperature and concentration are uniform and reactions occur simultaneously. To handle solid-gas reactions in this process, a R-Stoic block, CHAR-DEC, is set up before the series of RCSTRs. Char is decomposed into the elements C, H_2, O_2, N_2, S, and ash. The stoichiometric coefficients of these elements are determined according to the ultimate analysis of char, which is evaluated by a Calculator. The heat duty is specified as 0 in the specification sheet of R-Stoic in order to maintain the heat balance in the char decomposition.

The products leaving from CHAR-DEC enter a solid and gas separator, SEP-3. The separated gases, including H_2, O_2, and N_2 are introduced into the bottom of the gasifier together with the feedstock O_2 and H_2O. The separated solid components, including C, S, and ash, go to a series of RCSTRs to take part in the gasification and combustion reactions.

Each RCSTR has the same volume, which is equal to the whole gasifier volume divided by the number of RCSTR in the series. The heat loss between the bed and wall is represented by the heat stream. Each heat stream is bound with a Calculator and its value is determined by the corresponding Calculator. The Calculator automatically retrieves the reactor temperature in the flow sheet iteration and then updates the value of heat based on equation as follows:

$$Q_{loss}=-U\times A(T_{Reactor}-T_{Wall}) \quad (3.2)$$

Where Q_{Loss} = heat loss, Btu/ hr. U = heat transfer coefficient, Btu/hr·ft_2·°R.

3.6.4 Char Reactions

Char Partial Oxidation Reaction

$$C+\frac{Z+2}{2Z+2}O_2 \rightarrow \frac{Z}{Z+1}CO+\frac{1}{Z+1}CO_2 \text{..} II$$

Water Gas Reaction

$$C+H_2O \rightarrow CO+H_2 \qquad \Delta H=+131 \text{..............................} III$$

Boudourd Reaction

$$C+CO_2 \rightarrow 2CO \qquad \Delta H=+172 \text{..............................} IV$$

Methanation Reaction

$$C+2H_2 \rightarrow CH_4 \qquad \Delta H=+206 \text{..............................} V$$

CO – Shift Reaction

$$CO+H_2O \leftrightarrow CO_2+H_2 \qquad \Delta H= \ -41 \text{...............................} VI$$

Hydrogen Combustion Reaction

$$H_2+0.5O_2 \rightarrow H_2O \qquad \Delta H=-242 \text{..............................} VII$$

The parameter Z can be evaluated using this correlation by specifying pyrolysis temperature [9].

$$Z=\frac{[CO]}{[CO_2]}=2500e^{-\frac{6249}{T}} \qquad (3.3)$$

Where, Z is compressibility factor, [CO] & [CO_2] are mean concentration and T is the temperature in K [9].

3.6.5 Reaction Kinetics

Reactions (II-V) are the solid-gas reactions involving solid carbon as reactant in char with gasifying medium [10]. Some of these reactions are volumetric reactions, while others are surface reactions. In the volumetric reactions, gas can quickly diffuse into the particles and reaction takes place throughout the interior of particle as diffusion rate is much more as compared to the reaction rate [2]. In the surface reaction, gas does not penetrate into the pores and spaces inside the particle, but rather is confined at the surface of the shrinking core of unreacted solid [11]. Generally, volumetric reaction occurs when a chemical reaction is slow compared with diffusion. Surface reaction occurs when a chemical reaction is very fast and diffusion is the rate-limiting step [6]. Among these four reactions, the rate of reaction (II) is fast compared to the diffusion rate of reactants, so the reaction (2) occurs spontaneously on the surface of solid particles of char. The rates of the other reactions are rather slow compared with the reaction (2) because of the low operating temperature in the moving bed coal gasifier, typically lower than the ash fusion temperature. So, reactions (3-5) are volumetric reactions.

Based on the above explanation, the unreacted-core shrinking model is applied to describe the reaction rate of reaction (2) [7, 11]:

$$R_{co_2} = \frac{p_{o_2}}{\left(\frac{1}{k_{film}} + \frac{1}{kY^2} + \frac{1}{k_{dash}}\right)} \tag{3.4}$$

$$R_{C-O_2} = \frac{p_{O_2}}{\frac{1}{k_{film}} + \frac{1}{k_{dash}}} \tag{3.5}$$

$$k_{film} = 0.292 \times 4.26 \times \frac{\left(\frac{T}{1800}\right)^{1.75}}{d_p T} \tag{3.6}$$

$$k_{ash} = k_{film} \times \varepsilon_p^{2.5} \times \frac{Y}{1\text{-}Y} \tag{3.7}$$

Where, Rco_2: reaction rate, mole/cm^3·s, k $_{film}$: gas film diffusion coefficient, mole/cm^3·atm·s k $_{dash}$: ash diffusion coefficient, mole/cm^3·atm·s, P_{O2}: partial pressure of oxygen, atm. Y: r core /r particle.

After the drying and pyrolysis zones, the char produced moves to the gasification zone where it reacts with high temperature gasifying agents /medium (steam, hydrogen and carbon dioxide). In addition, the methanation shift (5) and carbon monoxide shift reactions (6) are also taken into account in the present gasification model. Char gasification involves a number of endothermic reactions which produces combustible gases such as CO, H_2 and CH_4.

After gasification, char still left behind flows to the combustion zone where combustion reactions (7) and carbon monoxide shift reaction (6) occur. Char partial oxidation (2) is a major reaction taking place in the combustion zone, which generates almost all the heat required for endothermic reactions. Finally the inert unreacted ash and char moves down into the ash zone. This unreacted char and ash is then removed by grater and ash lock hopper. It is assumed that negligible reactions take place in the inert ash zone at the bottom of gasifier. Their chemical reaction rate expressions and corresponding reaction rate constants are given in the table below:

3.6.6 Reaction Rate Expression For Char Gasification And Combustion

Table 3.2 Reaction Rate Expression

Reaction	Reaction rate	Comment	Unit	Source
3	$930e^{-\frac{45000}{1.987T}}.[c].(p_{H_2O}-p^*_{H_2O})$	$p^*_{H_2O}=\frac{p_{H_2}.p_{CO}}{e^{17.29-\frac{16330}{T}}}$	mole/cm^3·s	[11]
4	$930e^{-\frac{45000}{1.987T}}.[c].(p_{CO_2}-p^*_{CO_2})$	$p^*_{CO_2}=\frac{p^2_{CO}}{e^{20.92-\frac{20280}{T}}}$	mole/cm^3·s	[11]
5	$e^{-7.087-\frac{8078}{T}}.[c].(p_{H_2}-p^*_{H_2})$	$p^*_H=\left[\frac{p_{CH_4}}{e^{-13.43+\frac{10100}{T}}}\right]^{0.5}$	mole/cm^3·s	[11]
6	$Fw \times 2.877 \times 10^5 \cdot e\frac{27760}{1.987T}$ $\cdot\left[x_{CO}\cdot x_{H_2O}-\frac{x_{CO}\cdot x_{H_2}}{k_{wgs}}\right]\cdot p_t^{0.5-\frac{p_t}{250}}\cdot e^{-8.91+\frac{5553}{T}}$	$k_{wgs}=e^{-3.6890+\frac{7234}{1.82T}}$	mole/s· g of ash	[11]
7	$8.83x10^5e^{-\frac{9.976x10^4}{8.1315T}}C_{H_2}\cdot C_{O_2}$	--------	mole/m3·s	

Summary

In this chapter, model formation is discussed in detail. Details of each block and zone are mentioned. Physical property methods used in the model with component specification and process flow diagram are enlisted. The individual block description is mentioned in the latter part with the detail reaction kinetics of all the reactions taking place in gasification and combustion zone.

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CHAPTER 4

RESULT AND DISSCUSION

A simulation model for moving bed gasifier which was developed by Aspentech is used for this study. The model is being used for parametric analysis of bituminous and lignite coal. Coal data used in the model for lignite is retrieved from the literature and for bituminous the coal feed analysis and operating conditions are taken from Wen et al [1].

4.1 Parametric Analysis

Devolatalization/pyrolysis is the second step in the moving bed gasifier. It is a process in which coal is transformed at elevated temperatures to produce gases, tar, and char [2]. Devolatalization step determines the composition of tars in the product gas in a moving bed gasifier. The composition of product gases after pyrolysis process largely depends on the coal quality, temperature, heating rate, and pressure. Low rank coal like Thar lignite has relatively larger percentages of volatile matter and release large amount of gaseous products and less amount of tar as compared to higher rank bituminous coal [3]. Suuberg et al [4] studied the effect of temperature on the volatile yield during the coal pyrolysis for low rank coal having high percentage of oxygen in the ultimate analysis. He concluded that the yields of the volatiles increase exponentially with the temperature. He also investigated the effect of pressure on the composition of product gases. Vacuum pyrolysis of coal produces higher yields of heavy hydrocarbons and lower yields of light gases than are obtained in atmospheric conditions. Gibbins-Matham and Kandiyoti [5] found an increase in volatile yield in three of the four coals tested when the heating rate was increased from 1 K/s to 1000 K/s. For Pittsburgh no. 8 coal, one of the three coals that saw an increase in volatile yield, he concluded that the increase was mainly due to increase in tar production at a higher heating rate. The larger particle size tends to slow down heat and mass transfer rates and reduce the overall reaction rates and affect the quantity and quality of the product gases [6].

4.1.1 Optimization Of Pyrolysis Zone Temperature Using Bituminous Coal

Pyrolysis block temperature is varied for optimization at a constant steam to coal mass ratio and oxygen to coal mass ratio. Maximum hydrogen and carbon monoxide in product gas were achieved at 1500 K. The product outlet gas temperature is 989.99 K. Steam to coal mass ratio is 3.2 and oxygen to coal mass ratio 0.6. Product gas mass enthalpy= 8.64MJ/kg.

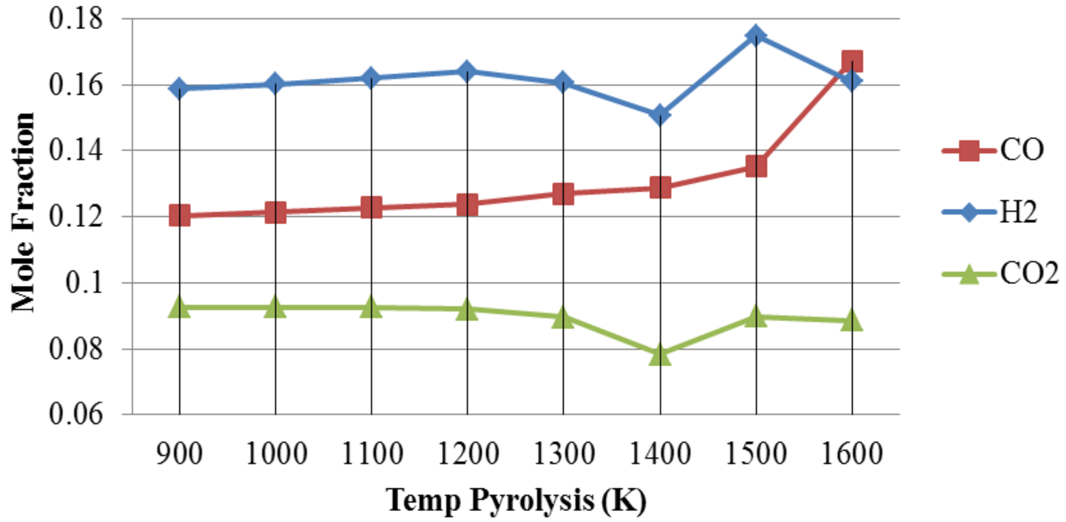


Figure 4.1 Mole Fraction of Syngas Major Components.

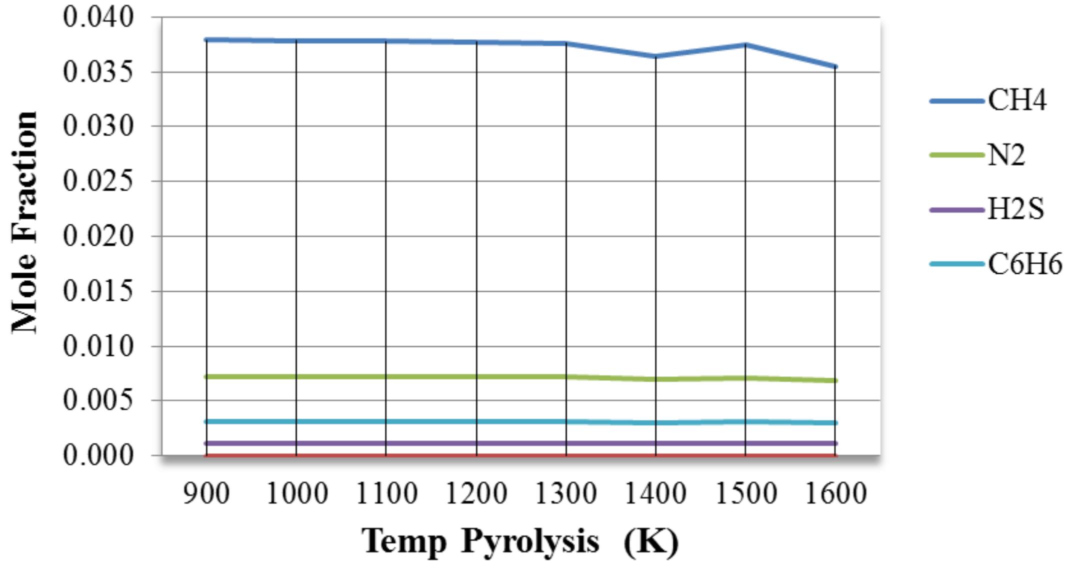


Figure 4.2 Mole Fraction of Syngas Minor Components.

4.1.2 Optimization Of Pyrolysis Zone Temperature Using Lignite Coal

Pyrolysis block temperature is varied for optimization at a constant steam to coal mass ratio and oxygen to coal mass ratio. For lignite coal S/C ratio and O/C ratio is kept lower for parametric analysis as coal feed already contains more oxygen and moisture in elemental analysis. Maximum hydrogen and carbon monoxide in product gas was achieved at 1400 K. The product outlet gas temperature is 1009 K. Steam to coal mass ratio is 1.48 and oxygen to coal mass ratio 0.4 Product gas mass enthalpy= 7.5MJ/kg.

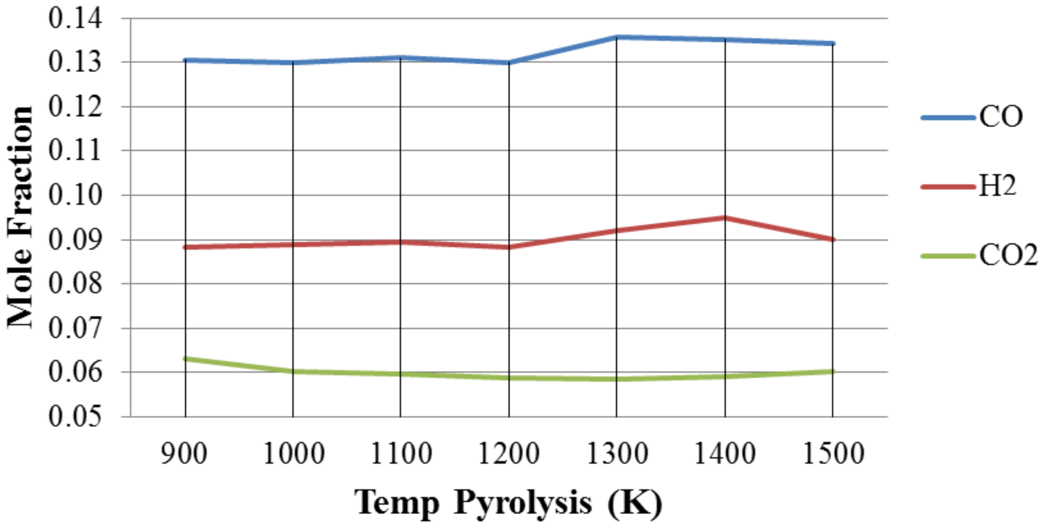
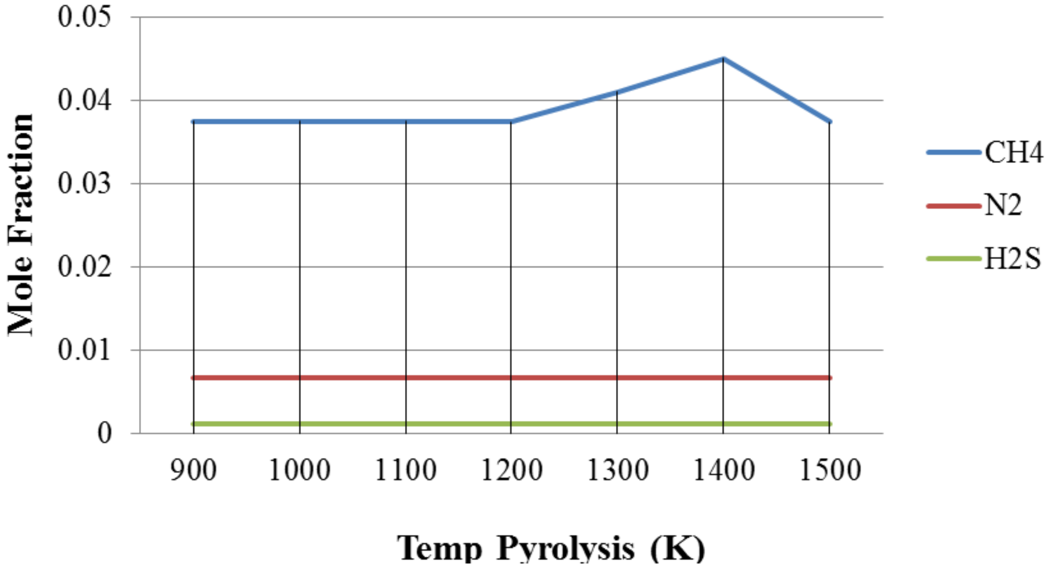


Figure 4.3 Mole Fraction of Syngas Major Components



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4.1.3 Optimization Of Steam Flow Rate Using Bituminous Coal

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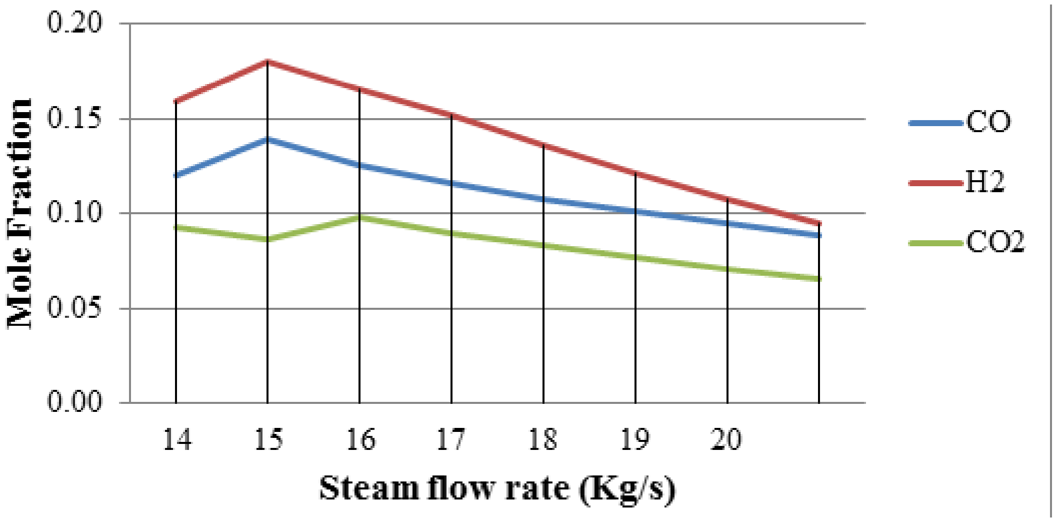

Figure 4.5 Mole Fraction of Syngas Major Components

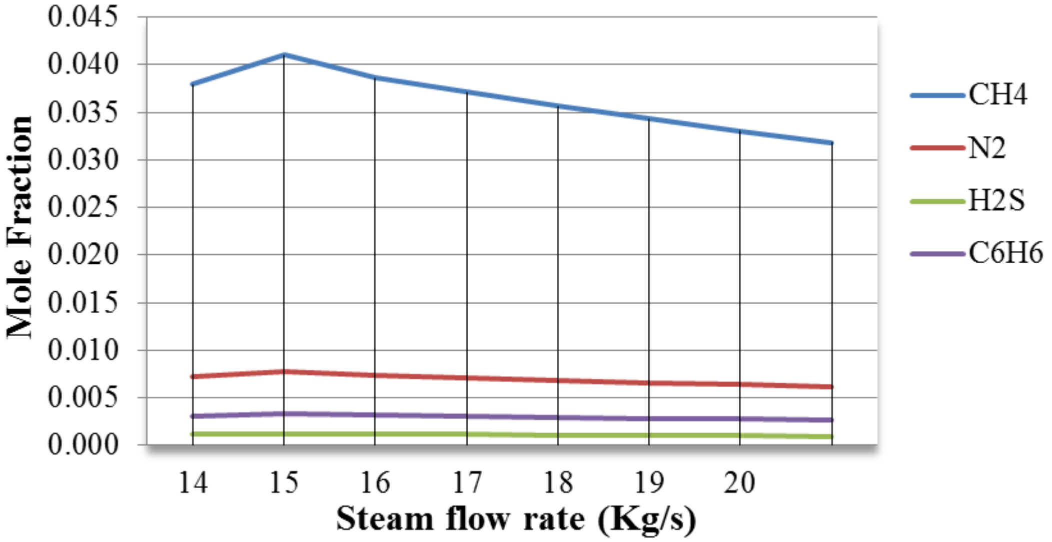

Figure 4.6 Mole Fraction of Syngas Minor Components

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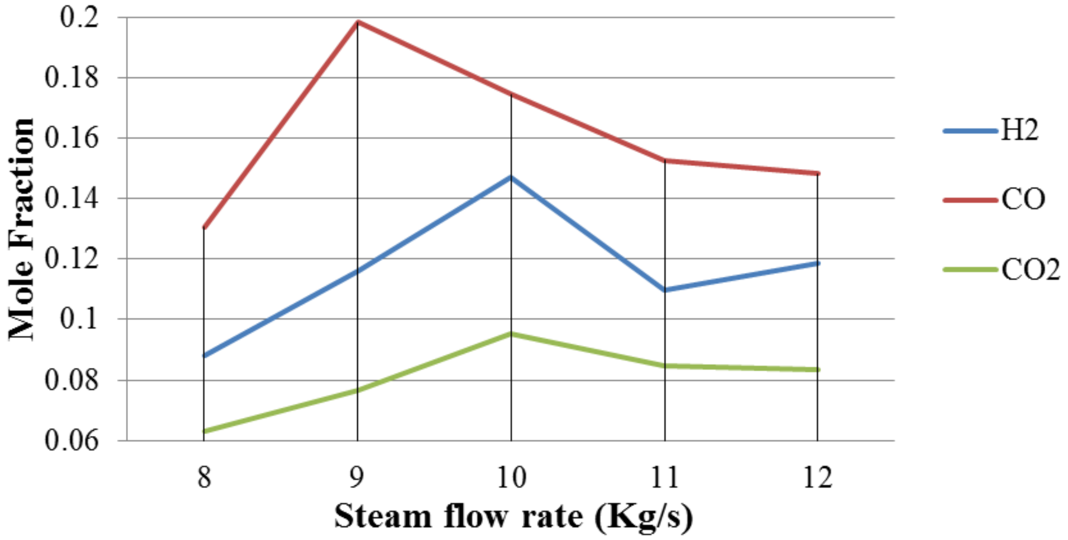

Figure 4.7 Mole Fraction of Syngas Major Components

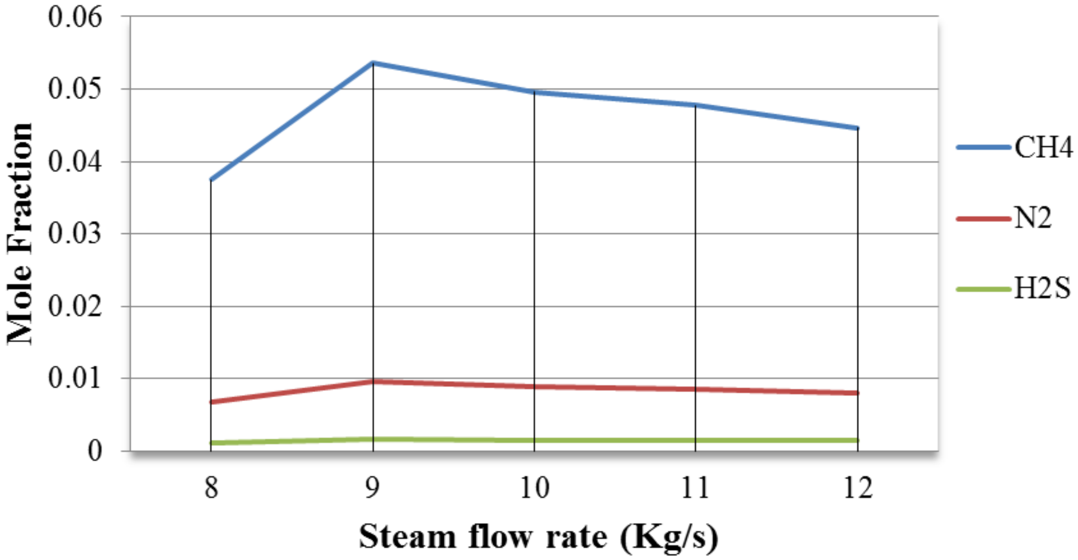

Figure 4.8 Mole Fraction of Syngas Minor Components

4.2 Syngas Component Profile For Lignite Thar Coal

Lignite Thar coal is being used as feed in the gasifier model at S/C mass ratio of 1.48 and O/C mass ratio of 0.4. Pyrolysis zone temperature is 900 K. Top to bottom profile of individual components were studied at above mentioned conditions of feed and temperature throughout the gasifier height which includes gasification and combustion zone.

4.2.1 Profile Of Gaseous Components

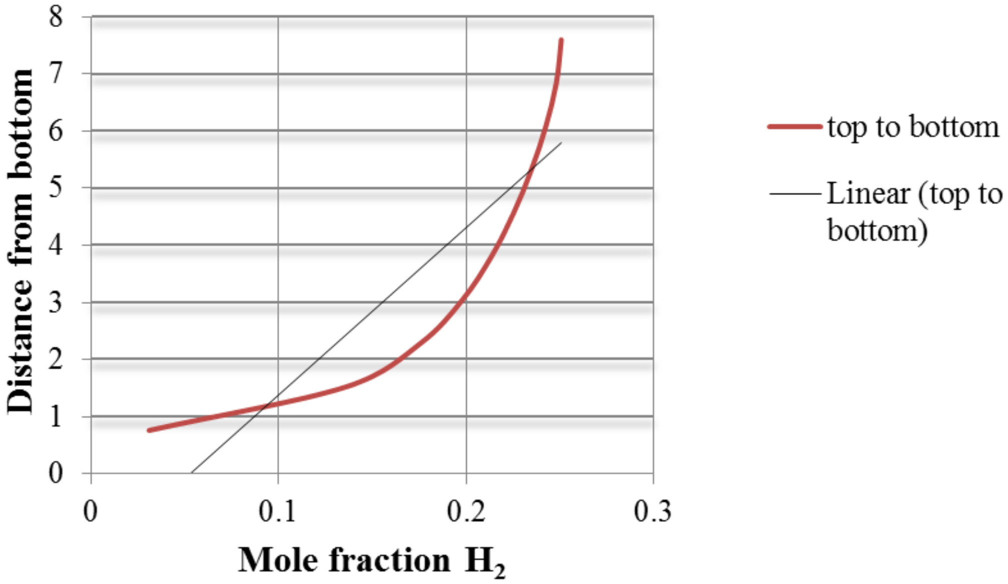

Figure 4.9 Profile Of H_2 From Top To Bottom

Maximum mole fraction of hydrogen (H_2), carbon dioxide (CO_2) and carbon monoxide (CO) is at the top of gasifier in gasification zone.

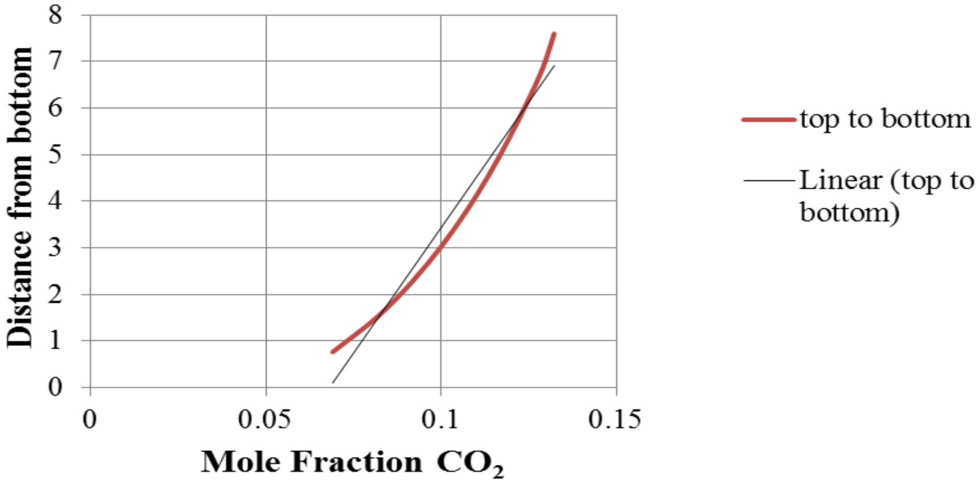

Figure 4.10 Profile Of CO_2 From Top To Bottom.

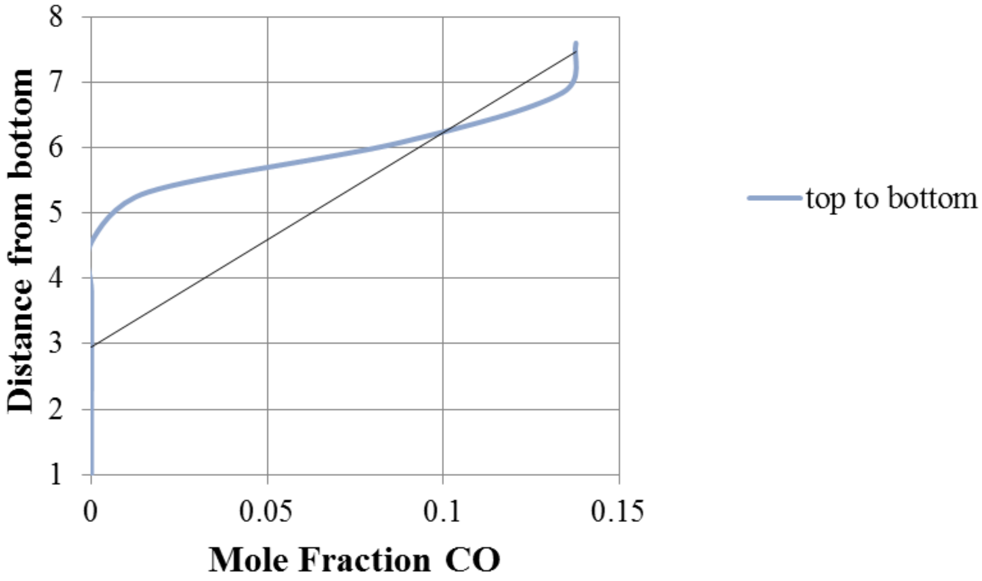

Figure 4.11 Profile Of CO From Top To Bottom

As shown in the above graph, carbon monoxide (CO) is negligible in the lower half of gasifier. This refers to the high temperature in the combustion zone resulting in high value of factor Z. Complete combustion of char takes place in this part of gasifier consuming most of oxygen supplied as gasifying medium from the bottom of gasifier.

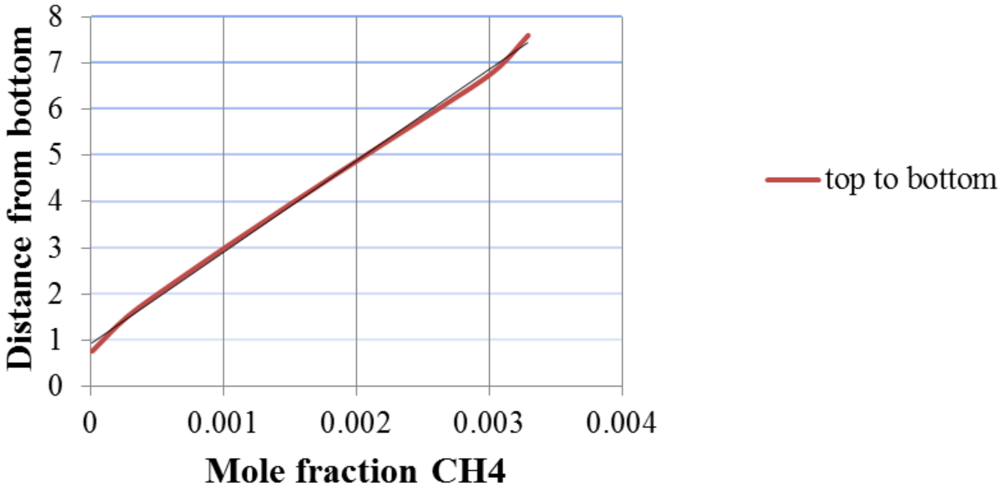

Figure 4.12 Profile Of CH_4 From Top To Bottom

4.2.2 Profile Of Solid Unreacted Char And Sulfur

Inert ash along with inconvertible char is collected at the bottom of gasifier with moving grater in dry form as operating temperature in the gasifier is below ash fusion temperature, resulting in a dry non-slagging process. Coal solid flow rate is maximum at the top in gasification zone and minimum at the bottom in combustion zone. Sulfur is minimum in lignite Thar coal and is assumed to convert only in hydrogen sulfide H_2S.

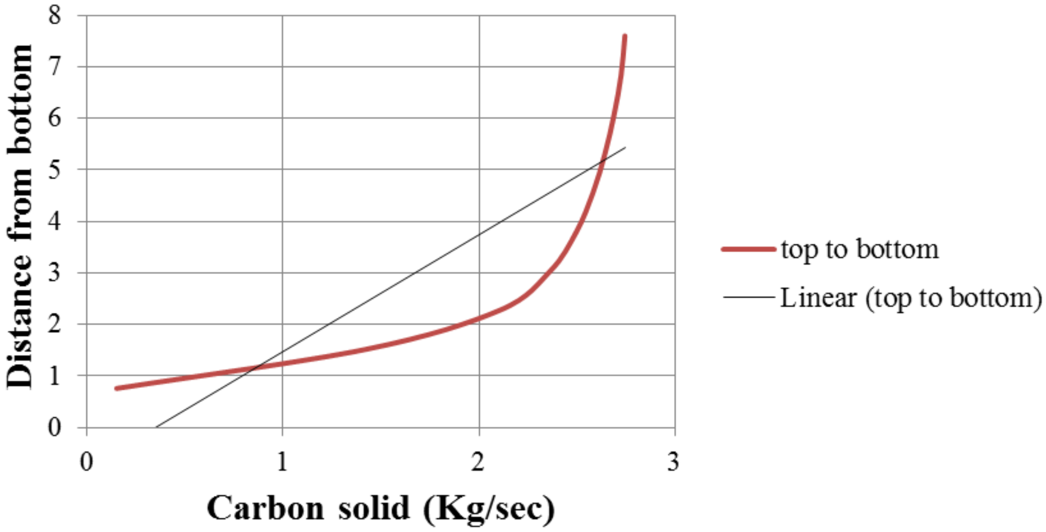

Figure 4.13 Distribution of Solid Carbon From Top To Bottom

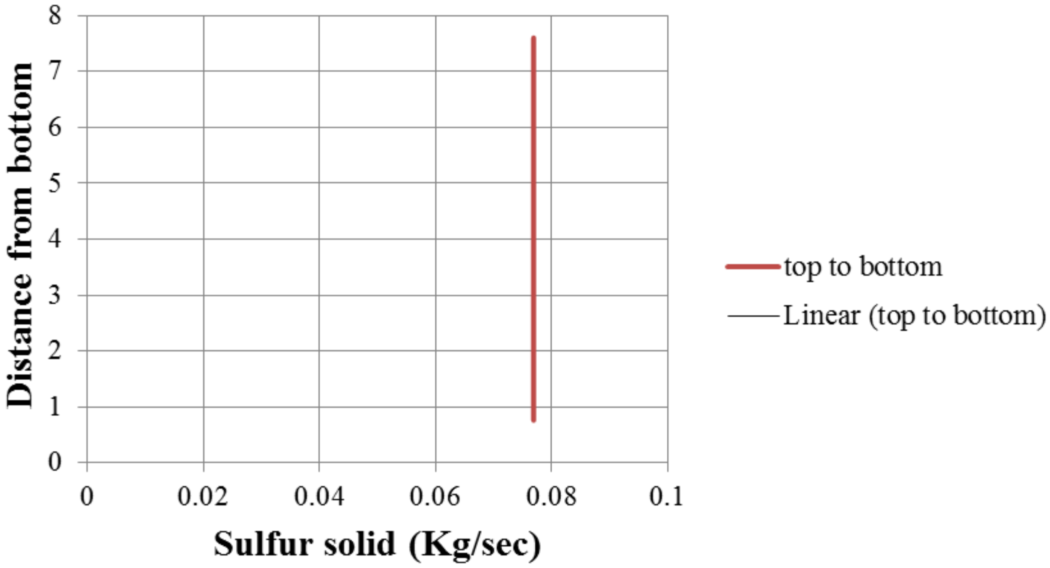

Figure 4.14 Distribution of Sulfur from Top to Bottom.

Summary

In this chapter results of parametric analysis done by using bituminous coal and lignite coal in the moving bed gasifier model were mentioned. The effect of pyrolysis zone temperature and steam flow rate of syngas composition is discussed. The optimized values of the S/C mass ratio and pyrolysis zone temperature are determined and discussed. For lignite coal, the individual components profiles of syngas at defined conditions were mentioned and discussed briefly.

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CHAPTER 5

CONCLUSIONS AND RECOMMENDATIONS

- Bituminous coal at high pyrolysis zone temperature yields an appreciable amount of H_2, CO & CO_2 (major components) in syngas.
- For the same amount of feed coal gasifying medium (steam, oxygen) required for the gasification of bituminous and lignite Thar Coal are different.
- Lignite Thar coal proves to be an attractive energy prospect after removal of excessive moisture.
- Oxygen required for gasification is less for lignite Thar coal.
- Medium BTU syngas is achieved from lignite, when gasifier is operated at low Steam/Coal and Oxygen/Carbon mass ratios.
- Lignite coal gasification produces a high heating value which can be further purified for hydrogen or can be used as precursor for methanol production.
- S/C mass ratio determines the operating temperature inside the gasifier and for lignite it should be kept lower because of the high reactivity of coal feed.
- The O/C mass ratio for Thar lignite is also less as compared to the bituminous coal.
- To make the process more energy extensive heat recovery in the waste heat boiler should be made effective and also the heat loss between the bed and the reactor all should be minimized.
- As lignite contains a large percentage of moisture so it is preferred to gasify this type of coal in dry ash Lurgi gasifier operating at temperature below ash fusion temperature.

Optimization of Process Conditions for Production of High BTU Value Syngas by Simulation Model of a Moving Bed Gasifier

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Abstract

Production of syngas by gasification of locally available coal in moving bed gasifier is one of the most economical and promising options to produce high calorific value gaseous fuel. Syngas contains significant amounts of C_1—C_4 hydrocarbons. Regarding the current situation of energy crisis and increase in the cost of conventional fuels (i.e. furnace oil) biomass and coal seems to be a cheap and accessible fuel in this part of the world. In these prevailing circumstances, syngas from surface mined coal gasification could be suitable alternate for limited natural gas. A moving bed gasifier designed by Aspentech in 2010 has been used to get some important results using local lignite coal samples, which are helpful in analyzing the potential of this conventional fuel. For this study, Aspen-Plus V8.0 has been utilized to simulate the performance of gasifier. The gasifier can withstand the temperature of 950°C and pressure of 3.5MPa. Several numbers of RCSTRs are used to specify gasifier in the model, which utilizes 5 kg/s of coal after drying and pyrolysis. In this study steam is used as a gasifying medium.The R-yield reactor is used for pyrolysis in the modeling. Particle size distribution (PSD) is not considered in the model and coal feed is assumed to be pretreated to remove excessive moisture to 5 % in the proximate analysis for the simulation in gasifier. Fortran Subroutine codes built in the model were used for obtaining the mass and energy balances for the different process steps within the syngas production process. Sensitivity analysis and process optimization is done by considering pyrolysis temperature and S/C ratio as input variables. Based on this investigation, critical process steps for process heat integration and syngas yield are identified.

KEYWORDS: Syngas, Pyrolysis, Particle Size Distribution, Moving Bed Gasifier

1. Introduction

Lignite Coal Resource located in the South Western Region Pakistan has a significant potential to play role in economic and energy sector. Coal recovered by open cast mining can be used in the local industries as cheap fuel providing energy mainly in cement and chemical processing plants [1]. Synthesis gas produced from gasification can be further used to produce liquid hydrocarbon fuels like synthetic diesel. The coal rank is lignite B with an average heating value of 5,333 Btu/lb and sulfur content of 1.57 % and ash content of 8.83 percent. The dry and ash-free heating value for the lignite coals is 12,322 Btu/lb [1, 2].

Moving bed coal gasifier is a vertical reactor. In dry ash gasifier, coal feed particle size is between 1.5-4 inch mesh screen that reacts easily with steam and oxygen in a moving bed. Coal feed reacts with gasifying medium to produce the gas containing CO, H_2, CO_2, CH_4, and other hydrocarbons[3]. Coal is fed into the hopper at the top of the gasifier and moves downward due to gravity. Oxygen and steam is introduced at the bottom of the pressurized gasifier. Four processes that take place in sequence from top to bottom: coal drying, coal pyrolysis, char gasification, and char combustion [4, 5].

Ash and unreacted char are removed by the rotating grate at the bottom, and the product syngas leaves at the top. Part of steam used in gasification chamber is produces by water jacket surrounding the chamber [4].

2. Model Description

In gasification model of coal drying and pyrolysis occurs instantaneously. This shows that Char gasification and combustion zone length is equal to almost the whole length of the gasifier. The moving bed coal gasifier is a countercurrent reactor. The countercurrent model is required to simulate combustion and gasification reactions of lignite coal, Aspen Plus no built in counter current reactor model which can be used effectively for parametric analysis [6]. Benjamin et al. developed a user solution program for the countercurrent moving bed coal gasifier, and then integrated it into Aspen Plus, but their results showed that the solution was time consuming. The form of the mathematical model of the countercurrent moving bed coal gasifier is a two-point boundary value problem. Its solution requires matching a number of variables, some specified at the top and others at the bottom of the gasifier. This feature causes the solution process to be usually complicated and time consuming. So, from the viewpoint of directly using the built-in algorithm in Aspen Plus and then simplifying the problem, a number of RCSTR reactors in series are proposed to model the char gasification and combustion processes [4]. The RCSTR reactor has the characteristic that all phases have the same temperature, which means the temperatures of solid and gas phases in the char gasification and combustion processes are equal in the model. CHAR-DEC, is set up before the series of RCSTRs. In this block, char is decomposed into the elements C, H_2, O_2, N_2, S, and ash. The stoichiometric coefficients of these elements are determined in accordance to their percentage in ultimate analysis of char. The heat duty in char gasification is 0 so that it does not alter the heat balance in the gasifier.Solid separator separates the products Char-Dec block into solid and gaseous streams, Sep-3. The gases separated are introduced with O_2 and steam, which are introduced from the bottom of gasifier. Solid components separated like carbon and sulfur enters into these series of RCSTRs to be gasified further and converted to CO and CO_2 [7]. The volume of RCSTRs used in the series is the same which sums up to the total volume of gasifier.The external Fortran code incorporated describes the reaction kinetics of all the gasification reactions occurring. Heat stream from each RCSTRS represents the heat loss between the reactor wall and the bed. Heat stream from each RCSTR is calculated individually. The reactor temperature in each iteration to converge model results is retrieved and heat stream is being updated accordingly.

The Bituminous and lignite coal used in the model for parametric analysis have proximate and ultimate analysis as shown in the table below:

Table1 Bituminous and Lignite Coal feed Analysis [1, 4]

Proximate Analysis (wt%)			Ultimate Analysis (Dry Basis .wt%)		
Element	Bituminous coal	Lignite Thar coal	Element	Bituminous coal	Lignite Thar coal
Moisture	4.58	5	C	77.6	67.6
FC	39.16	37.33	H	5.24	5.6
VM	52.72	47.82	N	1.47	0.91
Ash	8.12	14.85	Cl	0	0
			S	2.62	2.28
			O	4.79	16.4
			Ash	8.12	7.21

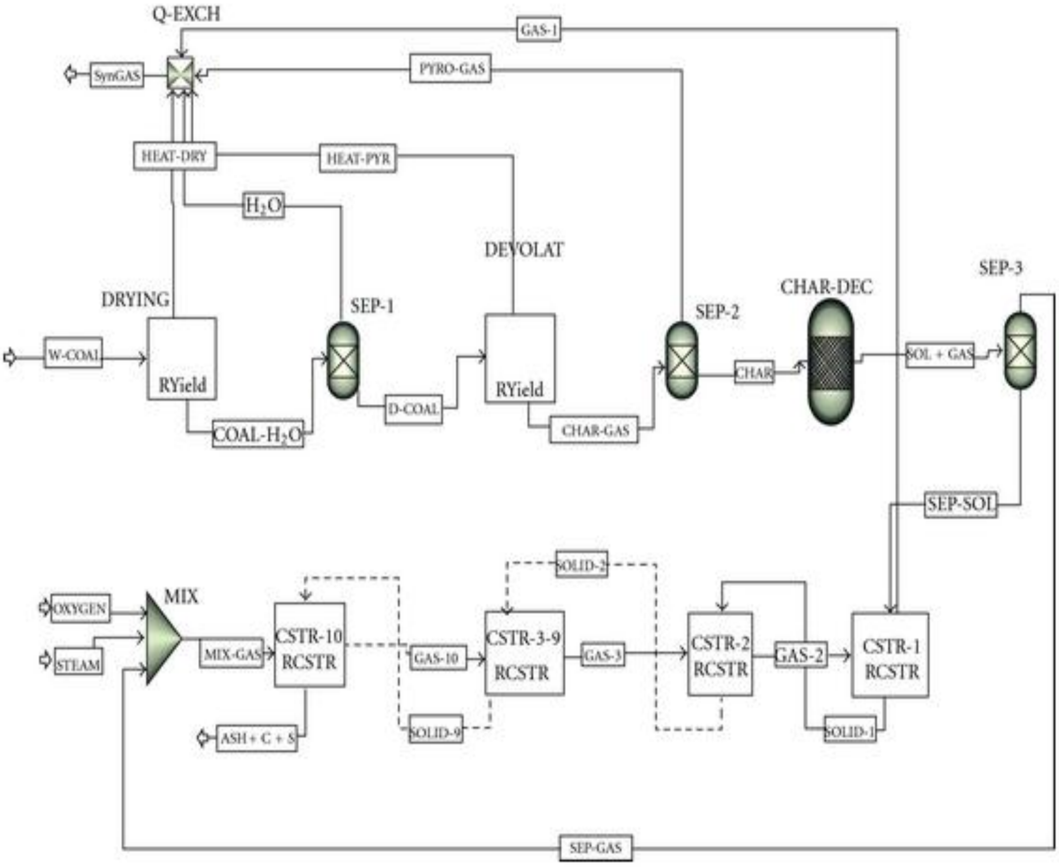

Figure 1 Block Flow Diagram [7]

3. Char Reactions

$$\text{Coal} \rightarrow CO + H_2 + CO_2 + H_2S + N_2 + CH_4 + C_6H_6 + \text{Char} \; \text{....(1)}$$

Char Partial Oxidation Reaction

$$C + \frac{Z+2}{2Z+2} O_2 \rightarrow \frac{Z}{Z+1} CO + \frac{1}{Z+1} CO_2 \text{..................................(2)}$$

Water Gas Reaction

$$C + H_2O \rightarrow CO + H_2 \qquad \Delta H = +131 \text{..............(3)}$$

Boudourd Reaction

$$C + CO_2 \rightarrow 2CO \qquad \Delta H = +172 \text{..............(4)}$$

Methanation Reaction

$$C + 2H_2 \rightarrow CH_4 \qquad \Delta H = +206 \text{..............(5)}$$

CO – Shift Reaction

$$CO + H_2O \leftrightarrow CO_2 + H_2 \qquad \Delta H = \; -41 \text{...............(6)}$$

Hydrogen Combustion Reaction

$$H_2 + 0.5O_2 \rightarrow H_2O \qquad \Delta H = -242 \text{..............(7)}$$

4. Results and Discussion

Devolatalization/pyrolysis is the second step in moving bed gasifier. It is a process in which coal is transformed at elevated temperatures to produce gases, tar, and char. Devolatalization step determines the composition of tars in the product gas in a moving bed gasifier. The composition of product gases after pyrolysis process largely depends on the coal quality, temperature, heating rate, and pressure [8]. Low rank coal like Thar lignite has relatively larger percentages of volatile matter and release large amount of gaseous products and less amount of tar as compared to higher rank bituminous coal. Suuberg et al studied the effect of temperature on the volatile yield during the coal pyrolysis for low rank coal having high percentage of oxygen in ultimate analysis. He concluded that the yields of the volatiles increase exponentially with the temperature[5]. He also investigated the effect of pressure on the composition of product gases. Vacuum pyrolysis of coal produces higher yields of heavy hydrocarbons and lower yields of light gases than are obtained at atmospheric conditions. Gibbins-Matham and Kandiyoti found increase in volatile yield in three of the four coals tested when the heating rate was increased from 1 K/s to 1000 K/s. For Pittsburgh no. 8 coal, one of the three coals that saw an increase in volatile yield, he concluded that the increase was mainly due to increase in tar production at higher heating rate. Larger particle size tends to slow down heat and mass transfer rates and reduce the overall reaction rates and affect the quantity and quality of the product gasesv[7].

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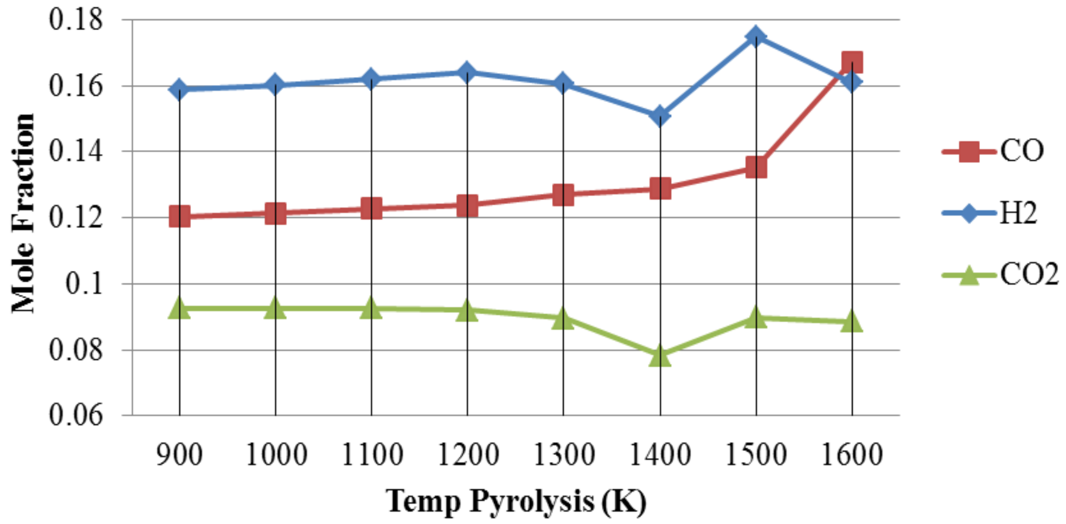


Figure 2 Mole Fraction of Syngas Major Components.

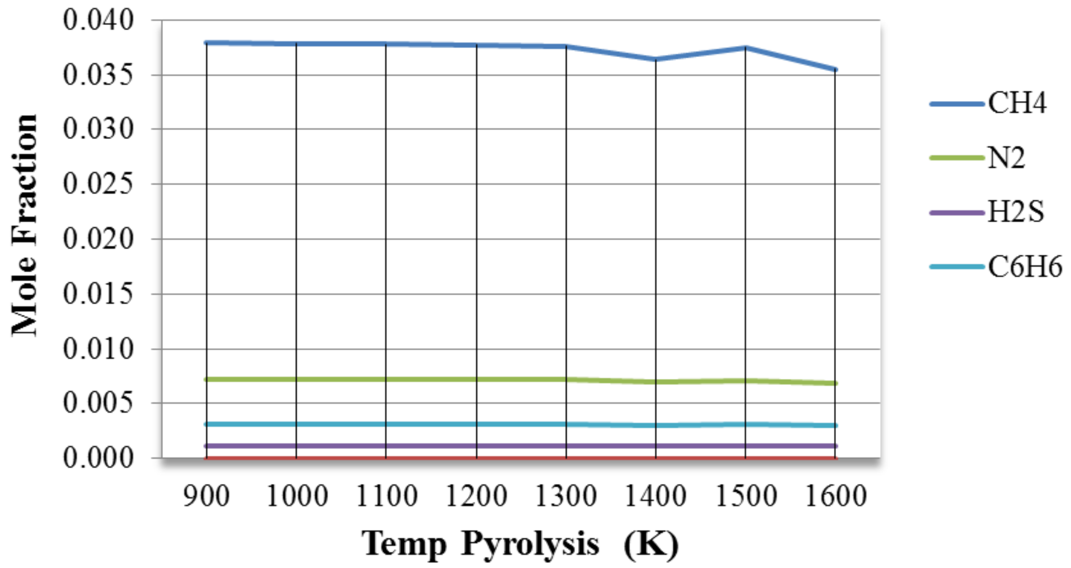


Figure 3 Mole Fraction of Syngas Minor Components.

Pyrolysis block temperature is varied for optimization at a constant steam to coal mass ratio and oxygen to coal mass ratio. For lignite coal S/C ratio and O/C ratio is kept lower for parametric analysis as coal feed already contains more oxygen and moisture in elemental analysis. Maximum hydrogen and carbon monoxide in product gas were achieved at 1400 K. The product outlet gas temperature is 1009 K. Steam to coal mass ratio is 1.48 and oxygen to coal mass ratio 0.4 Product gas mass enthalpy= 7.5MJ/kg.

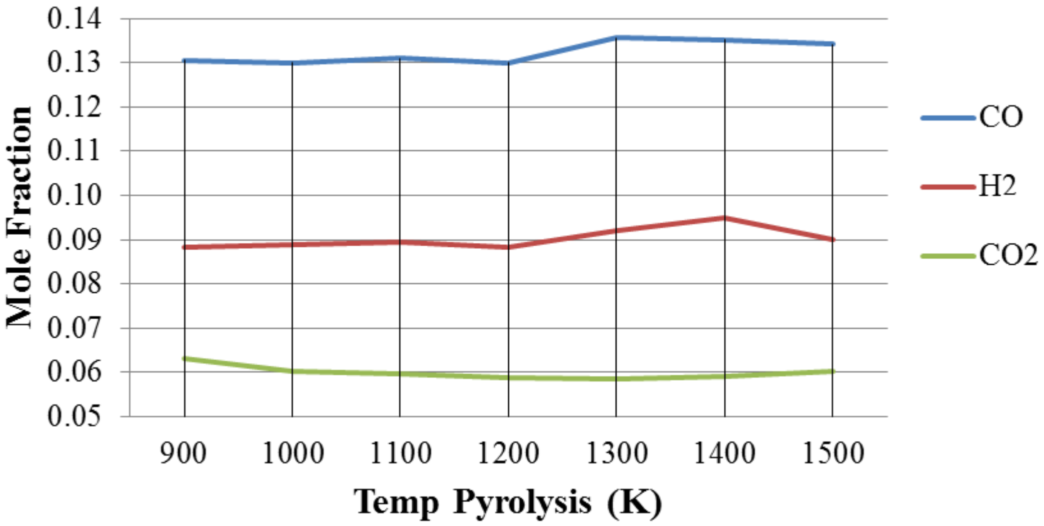
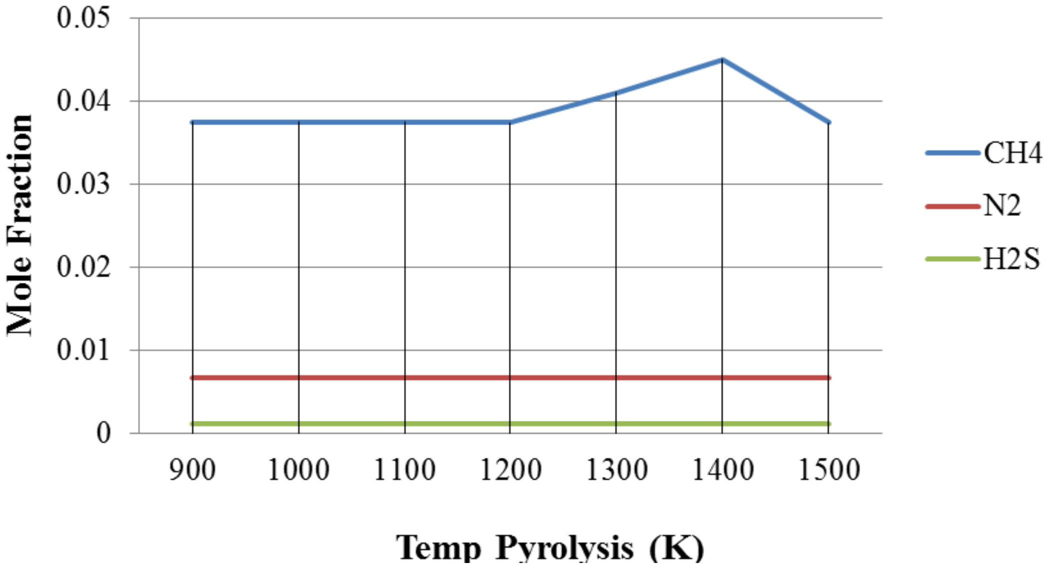


Figure 4 Mole Fraction of Syngas Major Components



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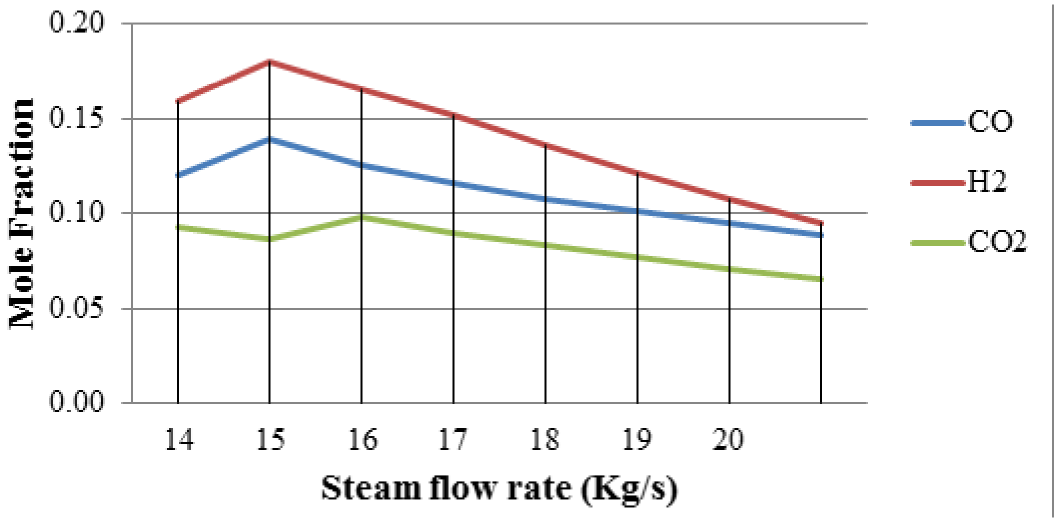

Figure 6 Mole Fraction of Syngas Major Components

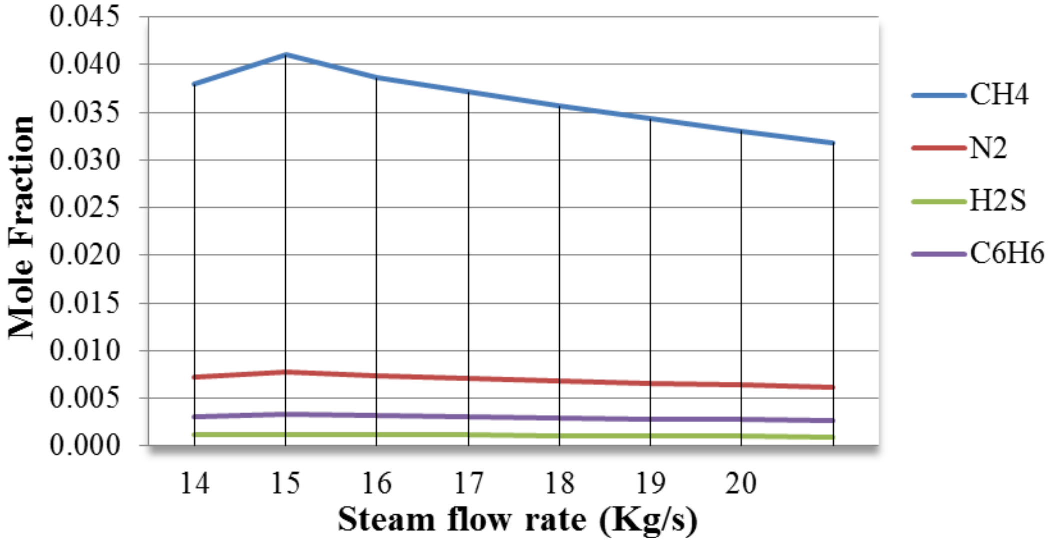

Figure 7 Mole Fraction of Syngas Minor Components

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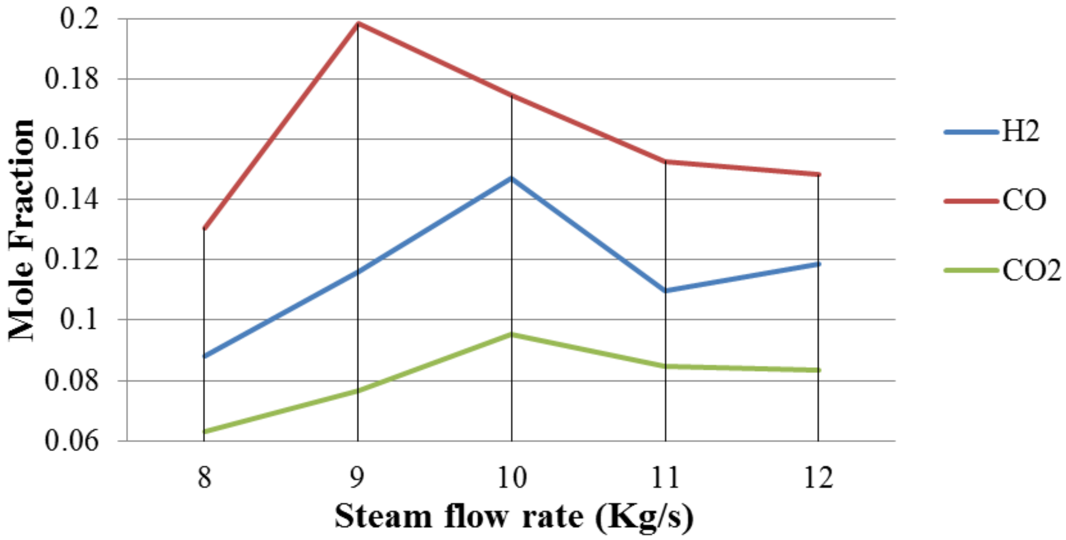

Figure 8 Mole Fraction of Syngas Major Components

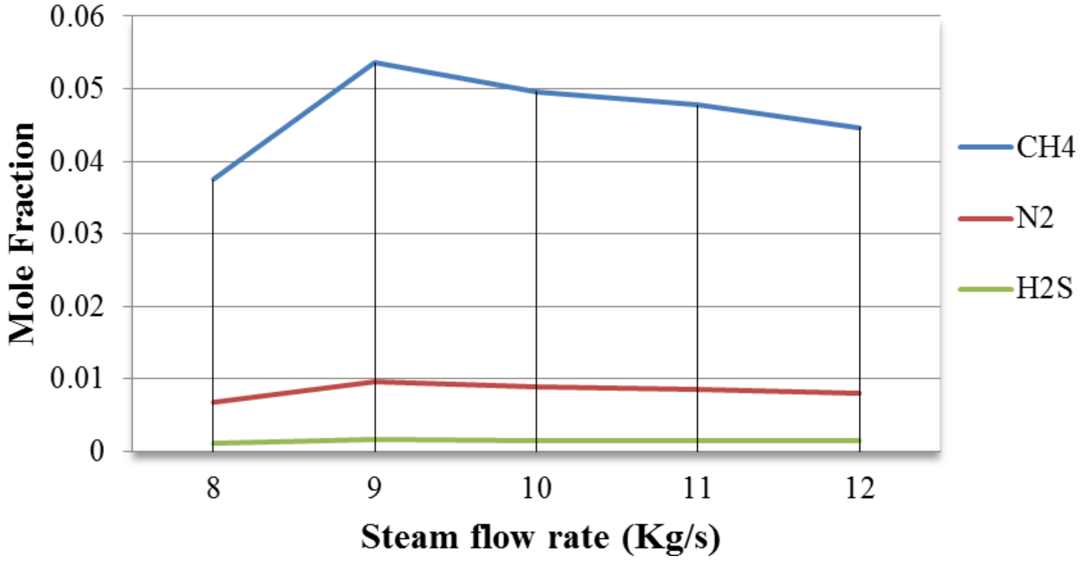

Figure 9 Mole Fraction of Syngas Minor Components

5. Conclusions

The optimum pyrolysis zone temperature for bituminous coal is 1400 K ad for lignite is 1300 K but at these high temperatures heat losses also increase appreciably.In case of S/Cmass ratio lignite is on the lower side as compred to bituminous coal. Bituminous coal at high pyrolysis zone temperature yields appreciable amount of H_2,CO & CO_2 (major components) in syngas. For same the amount of feed coal gasifying medium (steam, oxygen) required for gasification of bituminous and lignite Thar Coal are different. Lignite Thar coal proves to be an attractive energy prospect after removal of excessive moisture. Oxygen required for gasification is less for lignite Thar coal.

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Solid waste management and integration with modified Fischer Tropsch Synthesis Technology for utilization of MSW as an alternative renewable approach to produce green fuel

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ABSTRACT

Municipal solid waste is littered all over leading to insanitary living conditions. Per capita waste generation ranges 0.283-0.613kg/day 21.9 million MT annually in Pakistan.No serious efforts are made to adopt latest technologies of waste management, treatment and disposal. From the available routes, gasification of MSW to synthesis gas and thence to gasoline or diesel via fischer tropsch is quite promising from the standpoint of utilization of huge pile up of daily availablesolid waste material.Efficient energy technologies complementing renewable makes perfect research and business sense.Gasification is one of the leading-edge advanced technologies available to harness the production of syngas and thence high quality diesel using FTS and electricity generation.It takes every form of waste ranging from medical to elastomers, polymers and biomass of all kinds. The FT reactors converts waste components into syngas comprises of CO and H_2 which can either be converted into synthetic natural gas-SNG and diesel fuel via FTS or can be directly used in genset to provide electricity. The decision to implement any particular technology needs to be based on its techno-economic viability, sustainability, as well as environmentall implications. Keeping in view the local conditions and the available physical and financial resources, this technology is efficient competitive with minmal footprint would enhance corporate reputation for clean energy source producing synthetic diesel.

Keywords: Solid waste management, liquid oil, Fischer Tropsch Synthesis, Alternative approach, Syngas.

Introduction

Recent oil price hikes, energy supply security concerns, local air pollution, and global climate change provide incentives for introducing alternative energy carriers to petroleum products. One of the promising candidates is synthetic liquids produced by the Fischer–Tropsch (FT) process, which have received increasing attention worldwide due to technical advances and growing reserves of natural gas available at remote locations considered too small for liquefied natural gas (LNG) or pipeline projects [1]. Today, much of the interest in this technology is motivated by the desire of resource holders to monetize stranded gas reserves. Multi Tubular, Fluidized and slurry reactors are the commercially used designs for this purpose. The tubular fixed bed reactor (TFBR) has the distinctive advantage of not requiring separation of the product from catalyst and also the ease of scale up from one tube to thousands of tubes. It also has the highest possible catalyst loading per reactor volume and, therefore, has the highest potential of productivity per reactor volume. Plus, only the catalyst area near the inlet tube is affected by the reactants impurities while other areas remain fully functional. Furthermore, wax product can be easily separated from the catalyst. Still, heat removal in reactor requires attention for maximizing heavy hydrocarbons-HC production[2]. Considerable amount of literature has been found on TFBR modeling and design. Irani et al[3] used computational fluid dynamics as a technique to check the prediction of the reactor model using a novel iron catalyst. A 1D (one dimensional) heterogeneous model was applied by Wang et al[4] to study the performance of the fixed bed reactor. Atwood and Bennett[5] discussed parameter effects on commercial reactors using a 1D heterogeneous model. Mazidi and Sadeghi[6] researched on the maximum gasoline yield using non uniform catalysts in a one dimensional heterogeneous model. Guttel and Turek[7] compared slurry bed continuous reactor-SBCRs and FBRs on a 1D approach with cobalt based catalysts. Momonov and Kustov[8] investigated the effects of linear gas velocity and tube diameter using a 1D heterogeneous model Research has being carried out in Pakistan only on the practical preparation and performance of cobalt –based catalysts[9,10].Municipal solid waste (MSW) is a significant resource of renewable energy, and gasification technology is one of leading-edge advanced technologies available to harness production of syngas and thence high quality diesel using FTS & electric power generation with byproducts include steam, road making concrete & rock wool. Conversion of MSW to gaseous fraction is higher in plasma gasification compared to other technologies. Existing MSW know-how methodologies for conversion to energy have serious technological issues related to landfill for methane as an alternative energy resource. Fact of the matter is most of LFG projects are breakeven businesses because of generous incentives from technologically developed countries offer buy back warranties, CDM component, green technology financing schemes, high biodegradable MSW in urban areas, in order to make MSW a viable business[11]. In addition, amount and chemical composition of the produced gas depends on a variety of factors;

a) Huge footprint - Landfill site
b) Vast variation of waste composition organic portion in MSW, VOSCs
c) Ground water levels, risks of possible contamination by amount of landfill leachates
d) Climate temperature, wind, air pressure, etc.
e) Emplacement, landfill structure, design

Technological challenges for LFGTE

f) Low BTU, high inert portions (CO_2/N_2)
g) Leachate, Sulfur
h) Siloxanes = VOSCs

i) BTU variation from different parts of landfill site, Oxygen Content
j) Emission compliance
k) Capacity adaption, shift
l) Less experienced O&M staff

TABLE I: QUANTITY AND COMPOSITION OF WASTE MATERIAL COLLECTED VARIES DUE TO RAPID URBANIZATION:

Sr. no.	Type of waste material	Composition (%)
1	Coal	40
2	Municipal solid waste	25
3	Biomass (sawdust, wood, cloths, rice husk, wheat straws, cotton stems)	15
4	Waste tyres and polymeric waste	10
5	Medical waste	5
6	Plastics (PV, PET, HDPE, Nylon)	5

Possible sources of solid waste are domestic, transportation, water & waste water treatment plants, industries, botanical gardens, vegetable market, huge departmental stores, universities, slaughter house, agriculture and rural areas are shown in **Table I**.

Gasification is an emerging technology to convert MSW into clean, renewable, fuels which have commercial value.

The environmental impact of gasification is negligible compared to other forms of waste management. Landfills are toxic simmers that produce methane and leachate and represent operational & financial burdens. Incinerators produce dioxins and other harmful pollutants and have long been opposed because of serious impacts on eco-system. The decomposition of waste in landfills produces methane gas that contributes to climate change. Methane is estimated to have a global warming effect 23 times greater than carbon dioxide. This approach will also solve the issue of dumping MSW in landfills and save the community from harmful impacts.

Gasification which produces carbon dioxide instead of methane has a smaller impact on greenhouse effect than emissions from landfills. Society is additionally plagued with growing demand for energy, & traditional oil supplies cannot keep up with demand, especially when environmental concerns are becoming increasing important.

The calorific value, proximate and ultimate analysis along with the origin of various types of waste material is given in **Table II**.

TABLE II: CALORIFIC VALUE, PROXIMATE AND ULTIMATE ANALYSIS

Proximate analysis of MSW		**Ultimate analysis of MSW**	
Moisture	25%	Carbon	50%
Fixed carbon (db)	9.6%	Hydrogen	14.5%
Volatile (db)	55%	Nitrogen	2.5%
Ash (db)	10.4%	Chlorine	1%
		Oxygen	31.5%
		Sulfur	1.5%
Proximate analysis of biomass		**Ultimate analysis of biomass**	
Moisture	10-40%	Carbon	40-50%
Fixed carbon (db)	9-20%	Hydrogen	5-10%
Volatile (db)	25-30%	Nitrogen	0.5-2%
Ash (db)	2-10%	Sulfur	1-2%
		Oxygen	40-45%

Origin of waste	**Moisture Content (%)**	**Calorific Value (MJ/Kg)**
Paper	4-10	12-18
Coal	5-30	15-20
MSW	20-30	10-18
Biomass	10-40	16-20
Waste tyres & polymeric	1-2	12-19
Medical waste	2-8	15-22
Plastics	1-2	16-20

Gasification is a primary technology to enable carbon sequestration, because the carbon can be separated from the gasses and captured. It offers society the ability to address environmental and energy problems in a single solution. Thus utilizing waste for a renewable fuel enhances recycling, cleans the environment, and profitably produces valuable renewable energy.

The economics of gasification is very favorable because there are multiple revenue streams. Revenue is earned from collecting of MSW, sale of products and energy. The system makes money on the inputs and the outputs. It is an economically and environmentally attractive alternative to landfill. The bottom-line is a process based upon gasification technology for treating MSW thereby eliminating the need for landfill and can be used to process existing landfill MSW sites. FT converts syngas into diesel in a fixed bed reactor housing the catalyst and products separation is conducted down stream. At present Pakistan has a negligible R&D or HRD activity in this domain. Several programs are happening at various institutions/organizations with out any tangible results to date. The FT reactor is the key element in the production of syngas to diesel. With due diligence, in five years we should become experts at international level in design, production and control of

- FT reactors (For conversion of syngas to diesel)
- Development of catalysts
- Instrumentation & Control systems

To dispose of the municipal solid waste safely and in an environment friendly fashion, have become increasingly expensive and challenging for the communities. Mostly the MSW is dumped in low insecure spaces, rivers, oceans and other public places which are unnatural. If we keep in mind to recover the energy from it then gasification technology is well demonstrated commercial technology at work around the world but its application to waste discarding is limited. There are many processes for treating the waste but gasification is one of the most advanced technologies utilized for the purpose of getting some useful products [12]. Application of gasification technology in waste to energy, relieves the pressure on distressed landfills, and offers an environmentally caring method of disposing MSW. Even to get rid of plastics waste is of considerable social significance by using this technology. The plastic waste may be Polypropylene, Polystyrene, Polycarbonate, PVC, Nylon, HDPE, LDPE and acrylic fibers waste. It senses to be an economic and abundant source of energy, and a reliable source of power. Humanity is learning that mineral resources are not unlimited. Global oil production is unable to match rising demand for clean energy, and that is in turn leading to higher prices for gasoline and other fuels. It will embark on innovative concept addressing menace of municipal solid waste (MSW) effectively in contrast to inefficient renewable landfill gas. Emerging technologies such as gasification can process landfill waste to extract commodity recyclables & convert carbon-based materials into valuable fuels. Municipal solid waste gasification can form an integral component in the system to achieve zero-waste and produce renewable fuels while cleaning the environment.

In its purest form, incineration involves burning of organics in the presence of excess oxygen, converting them to heat, particulates, and a variety of combustion gases, with all of these vented to the atmosphere. Gasification has been in use since the late 1800s in the metal industry, expanding into the chemical industry in the 1900s. The gasification function on the principle that is lack of oxygen in waste decomposition prohibits combustion. Gasification is one form of the incomplete combustion of MSW for the purpose of obtaining a variety of gaseous, liquid, and solid products, including fuels, metals, and chemicals[13].

Experimental Setup and Catalyst Characterization

In present research work, cobalt supported on various ceramic supports like alumina, silica, titania, silicon carbide with promoter like potassium, sulfur, phosphorus is utilized. An assembly of FT bench scale facility having two single tube fixed bed bench-scale reactor was used with ID of 9 mm and tube length of 0.3m along with two separator units and online gas chromatograph is connected with the whole facility to find out the composition of reacting gases mixture and leaving gases mixture. Cobalt supported on alumina/silica doped with sulfur along with potassium as a promoter catalyst with the properties shown in **Table III** was placed in the middle of the reactor.

TABLE III CATALYST PROPERTIES

Property	**Unit**	**Content**
Alumina	Wt%	20
Silica	Wt%	20
Cobalt	Wt%	10
BET Surface Area	m^2/g	200
Diameter	Mm	2
Bulk density	kg/m^3	800

The quantitative analysis and SEM image done by Joel-SEM (JED2300) is given in **Table IV and Fig.1**.

TABLE IV QUANTITATIVE ANALYSIS

ZAF Method Standardless Quantitative Analysis				
Fitting Coefficient : 0.6265				
Element	keV	Mass %	Error %	Atom %
O	0.525	51.38	0.89	66.56
Al	1.486	17.15	0.57	13.17
Si	1.739	18.14	0.68	13.39
S	2.307	5.02	0.57	3.24
K	3.312	1.84	0.75	0.98
Co	6.924	5.25	2.29	1.85

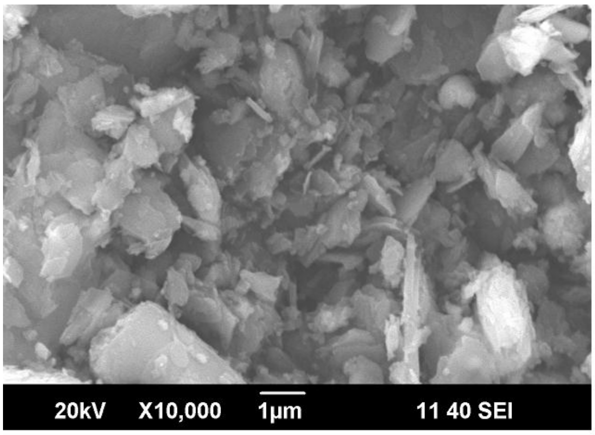


Fig.1 SEM image of $Co/Al_2O_3/SiO_2/S/K$ catalyst

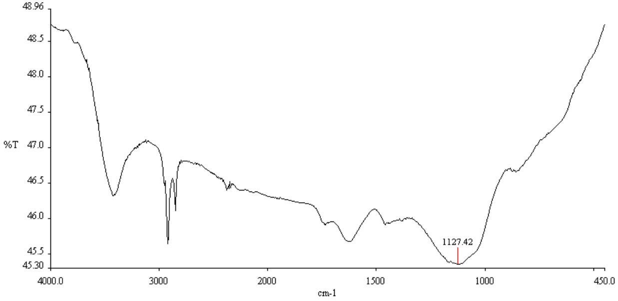
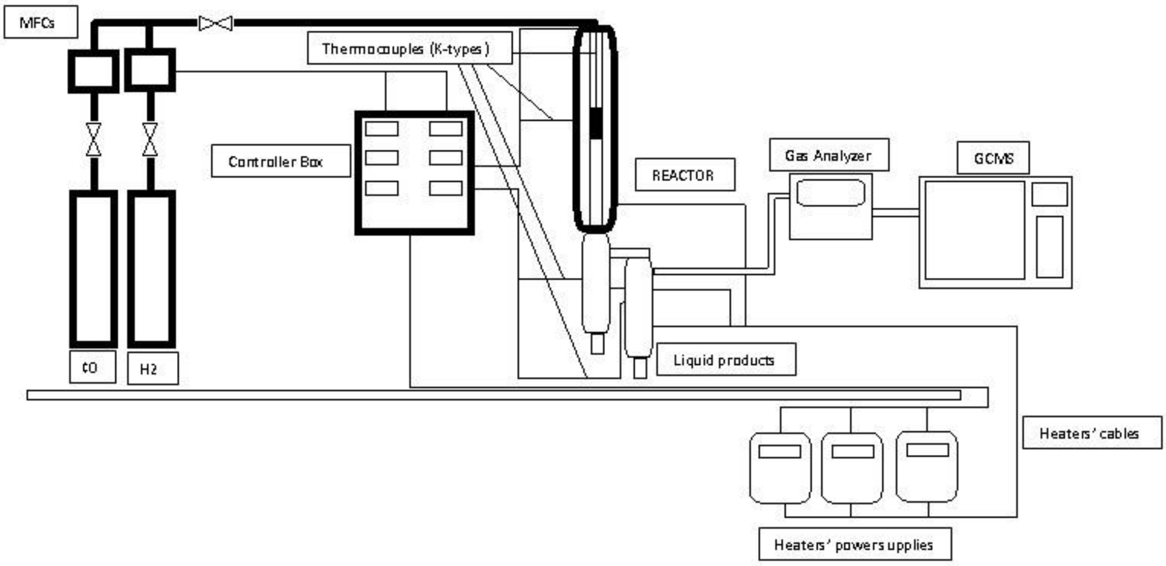


Fig.2 FTIR of $Co/Al_2O_3/SiO_2/S/K$ catalyst

The rest of the reactor was packed with ceramic balls and special type of cloth material.CO, H_2 flow was controlled through separate mass flow controllers (Sevenstar D07 MFC). Prior to the synthesis the catalyst went under reduction in H_2 for 16 h at 350°C at 0.4bar. Then the reactor was cooled down to 180°C and pressurized to 1bar. The synthesis gas from the gasifier can be fed to this facility because gasifier is not available. We used bottle gases like CO, H_2 and N_2 to make syngas mixture as required. The synthesis was started at 200°C with H_2/CO ratio of 2. A run time of 12 h for three runs with different GHSVs was conducted under constant pressure

Fig 3: Schematic diagram of bench scale fixed bed reactor system



and temperature. After leaving the reactor the products pass through two traps, one hot and one cold. The hot and cold traps separate the heavy and light hydrocarbons from the product stream respectively. The composition of synthesis gas is in the range of syngas expected to be produced from UCG of Thar coal reserves. Suspended solids are separated from the synthesis gas (syngas). Thus, no solids are assumed to be present in all downstream units, simplifying the model since only two fluid phases, liquid and vapor, are considered. The samples from each run were collected from the manual valves situated beneath the traps. Schematic diagram showing the flow and control of the gases and product is described in fig.3. Sample analysis was done on an offline GCMS. Temperature of the reactor was controlled by placing one thermocouple near the wall and the other in the catalyst bed. Pressure was controlled using a back-flow regulator. Reactor dimensions and operating conditions are outlined in **Table IV**.

TABLE IV: BENCH-SCALE REACTOR OPERATING CONDITIONS

Parameter	Unit	Value
Pressure	Bar	1
Wall Temperature	°C	200
Metal heat coeff.	$W.m^{-1}.K^{-1}$	45
Length	mm	300
ID	mm	9
OD	mm	11
H_2/CO		2
Space velocity	h^{-1}	230

Rate of reaction based on $Co/Al_2O_3/SiO_2/S/K$ catalyst. Since the catalyst used was cobalt no water-gas shift reaction is taken into account due to cobalt catalyst's negligible in-situ WGS activity and the H_2/CO ratio taken in this study being above 2. Since C1 and C2 compounds deviate from the ASF theory, it was used for higher HC whereas individual rate laws were given for the compounds mentioned above[13]. The temperature dependent constants were calculated according to the experimental results and the energies of activation were taken from the. available literature[14,15].

TABLE V: EXPERIMENTAL AND PREDICTED RESULTS 200°C, 1BAR

GHSV	**30Nml/g_{cat}.h**		**60Nml/g_{cat}.h**		**90Nml/g_{cat}.h**	
	EXP	PRE	EXP	PRE	EXP	PRE
X_{CO}%	10.2	10.9	6.9	7.5	4.5	4.9
X_{H2}%	13.4	14.1	9.7	10.5	6.8	7.2
S_{CH4}%	6.11	5.90	4.54	5.10	5.20	5.70
S_{C2}%	1.45	2.11	1.95	2.32	1.34	1.97
S_{C3}%	3.53	3.30	3.84	3.47	2.70	3.15
S_{C4}%	3.70	3.95	2.95	3.75	2.53	3.67
S_{C5+}%	85.2	84.7	86.7	85.4	87.2	85.5

Results and Discussion

Chemical composition of syngas produced by gasification of MSW/coal/biomass depends upon various operating conditions temperature, pressure, and catalyst used during this operation. The syngas yield, ratio of hydrogen and carbon monoxide, percentage of sulfur along with unwanted gases and LHV of the syngas can effects the conversion of syngas into liquid fuel by FTS. A number of wastes to energy technology utilization are applied for utilization of MSW. The economics of power generation can be enhanced by means of taking interest in the waste to liquid fuel technology. The combined burden of increasing quantities of wastes and environmental legislation in Pakistan that limits the wastes that can be disposed to landfill has lead to an increase in the number of thermal treatment plants operating on MSW. The greatest increase has been in the number of energy-from waste plants that treat municipal solid wastes (MSW). In urban areas of Pakistan, amount of MSW is increasing each year. Actual FT runs were performed using a single 28 mm ID tube. On a positive note, the system pressure drop remained within acceptable limits i.e. 0.03 MPa/m, in spite of the nano size. This compares favorably with systems involving macro size particles. The GCMS spectrum of the FT product cuts is presented in **Fig. 4** showing light (C5-C6) and heavy naphtha fraction (C7-C9) along with a dominant fraction of diesel fuel (C12-C20). The catalysts synthesized thus enables to get selective product yield of liquid hydrocarbons (C12-C20), falling in the range of diesel fuel. The wax (C21-C26) is recovered from the first stage of product refining as reflected in the GCMS spectrum.

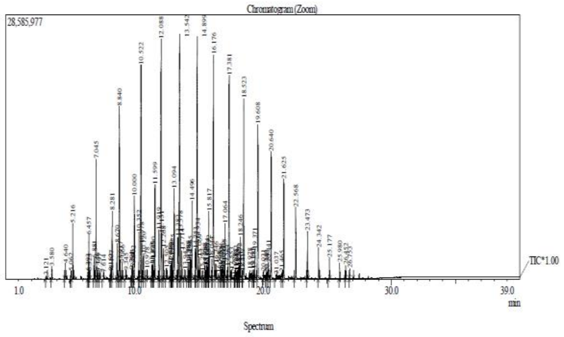


Fig. 4 FT Products distribution by GCMS

On the basis of material balance respective fractions of product cuts are reported in **table VI**, which compares product distribution with & without wax cracking.

TABLE VI FT PRODUCTS BASED ON SYNGAS

Sr. No.	FT-Products	With Catalytic Cracking of Wax	Without Catalytic Cracking of Wax
1	Liquid Petroleum Gas	0.145%	0.145%
2	Light Naphtha	9.328%	5.35%
3	Heavy Naphtha	27.115%	22.126%
4	Diesel Distillate	63.485%	22.487%
5	FT-Wax		56.255%

Table VII provides a comparison between conventional fuel and synthetic diesel produced by Fischer Tropsch technology. The fact that the products are predominantly straight chain hydrocarbons and contain very little aromatics, (unlike crude derived fuels) ensures that the fuel is clean burning with minimal soot formation.

TABLE VII: COMPARISON OF CONVENTIONAL CRUDE OIL & FT DERIVED PRODUCTS

S#	Property	FT derived diesel distillate	Crude derived diesel distillate
1	Density at 15°C (Kg/m^3)	772-808	841
2	Total aromatics (mass %)	0.3-0.7	39.4
3	Cetane number	>70	55
4	Sulphur (ppm)	<5	42
5	Flash point (°C)	60-72	>55
6	IBP (°C)	154-210	N/A

Conclusion

Considering exhaustible oil reserves and current hike in crude oil prices, there is a growing interest for preparation of hydrocarbon fuels from municipal solid waste, coal or biomass. From the available routes, gasification of coal to synthesis gas and thence to gasoline or diesel via Fischer Tropsch is quite promising from the standpoint of utilization of huge coal reserves present in Pakistan. The conversion of coal to alternative fuels could offer more environmentally acceptable process for energy production. Coal gasification refers to a process that breaks down coal into its components, by subjecting it to pressure and high temperature in addition to the use of steam and air/oxygen. This leads to the production of synthesis gas, which is mainly a mixture of carbon monoxide, hydrogen and traces of carbon dioxide, methane, and some other compounds depending upon quality of coal. Gasification is a vital process for the production of syngas ($CO+H_2$) chemical composition depends upon feedstock properties like volatile matter, fixed carbon, moisture.

To create an efficient technology pathway of syngas production through gasification which will provide an alternative to preserve natural gas for domestic consumption and as a raw material for higher value added products like fertilizers, synthetic fuel, pharmaceutical wax, electric power and petrochemical industry. On long term basis, this facility has a potential to produce a clean source of hydrogen for commercial applications. Coal gasifier capable of using enormous source of untapped energy in local coal will promote a phenomenal share to shrink the energy challenges of our industries. Clearly, the abundance and availability of coal makes it such a promising alternative energy source over natural gas or other fossil fuels. It is notable that abundantly available black gold is not being utilized properly up to the present time to meet energy demands of Pakistan..

The gasification of MSW/Coal/Biomass coupled with FTS processing leads to liquid fuels of different grades and compositions for commercial applications. The catalyst developed in-house shows adequate selectivity for the targeted diesel fuel fraction in the product stream. Developing indigenous R&D capabilities for adopting various advanced coal technologies to suit local conditions are the key purposes of this catalyst synthesis for FT synthesis technology.

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ABBREVIATIONS

TFBR	Tubular Fixed-Bed Reactor
LHV	Lower Heating Value
GHSV	Gas hourly space velovity
HC	Hydro-Carbon
FTS	Fischer Tropsch Synthesis

NOMENCLATURE

u_{sv}	Superficial velocity	($m.s^{-1}$)
ρ_B	Catalyst Bulk density	($kg.m^{-3}$)
C_p	Specific heat capacity	($J.kg^{-1}.K^{-1}$)
$-\Delta H$	Reaction Enthalpy	($J.kmol^{-1}$)
U	Heat Transfer Coefficient	($W.m^{-2}.K^{-1}$)
T_W	Wall Temperature	(K)
P	Pressure	(Bar)
d_p	Particle Diameter	(m)
R	Molar Gas Constant	(J/kmol.K)
λ	Thermal conductivity	($W.m^{-1}.K^{-1}$)
L	length	(m)

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