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Simulation of Steam Gasification of Coal with PreCombustion enabling Cleaner Coal Conversion

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Gasification is one of the cleanest possible ways to exploit abundant coal reservoirs all over the world to produce electricity and synthesize chemicals. Major challenges in the design of any gasification plant are desulfurization of the gases produced as a result of high sulfur contents in some coal types, removal of tar in the product gas, and costs associated with Air Separation Unit.

For environmental sustenance and energy saving, an indirect gasification scheme for coal is proposed and simulated which uses steam instead of oxygen-steam mixture as the gasification medium. This avoids the need of costly air separation process, while the heat for the endothermic process is supplied by hot flue gases passing through a bayonet heat exchanger installed within the reactor vessel. Simulation is carried out using the Aspen Plus™ software integrated with an MS Excel™ spreadsheet.

The simulation results show a remarkable achievement of cold gas efficiency of 70 %. The utilization of heating value of coal is optimized as the process is fully heat integrated and large amount of surplus superheated high pressure steam is generated providing for the electrical power needs of the installation.

The proposed gasification scheme can be used to convert high sulfur-containing coal to fuels, chemicals and energy in areas like Thar, Pakistan, where there are an estimated 175 billion tons of coal reservoirs with sulfur content as high as 2.9 wt. %.

1. Introduction

Increasing levels of greenhouse gases and the subsequent environmental impacts due to the fossil fuels based power generation and petrochemical industry has led to the consideration of minimizing the use of such fuels and switching to more environment friendly technologies. To consume the still vastly abundant fossil fuels among which coal is the most abundant and most evenly distributed around the globe (Emun et al., 2010) in the cleanest possible way, gasification serves as one of the most viable solutions with a number of technologies available varying with respect to configuration, capacity, feedstock, fuel flexibility and product gas requirement. Integrated Gasification Combined Cycle (IGCC) power generation is a promising technology for clean coal utilization but it comes with a number of challenges to be considered.

IGCC's wider commercialization is principally hindered by the effects of the efficiency and operating costs of Air Separation Unit (ASU) equipment, as mentioned by Fu et al. (2014). Secondly, sulphur content in coal leads to the production of sulphur containing gases threatening to the environment and the infrastructure. Pre-treatment of coal to remove sulphur has been studied by Fois et al. (2010) and Vaccaro (2010) using sequential leaching of sub-bituminous coals but this method involves the processing of the large solid volumes with long treatment durations. Otherwise, the entire volume of syngas generated with a little more than 1 vol. % sulphur compounds has to be cleaned (Sofia et al., 2013). A conventional syngas cleaning train would include scrubber, hydrolysis reactor, and MDEA absorber to remove sulphur compounds later sent to Claus process for conversion to elemental sulphur. Thirdly, tar presence in the syngas produced (depending on the gasification feedstock) causes operational problems downstream and must be removed using high temperature of gasification, higher oxygen flowrate or the use of catalysts (Pinto et al., 2007).

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Multiple studies on gasification have been performed on existing and novel technologies using process simulation algorithms and software to predict the behaviours of a proposed process scheme and/or reactor configuration. Lee et al. (2010) have reported the use of a singular reactor (RGibbs, RYield, or RStoic) to represent a gasifier in the evaluation of most of the gasification processes as recently done by Chen et al. (2012) and many others. Very few studies take into account a model for gasifier addressing the effect of temperature profile from the gasifier top to bottom.

This work is aimed to simulate an indirectly heated moving bed gasifier with a complete heat integration scheme. The coal feed is precombusted with hot air to remove the volatile components, tars and sulphur so that only char and ash are left for further processing in the gasifier. The combustion of sulphur in this stage produces H_2S which causes severe environmental implications and needs to go through downstream treatment, yet due to precombustion, the volume of gas to be treated is much less as compared to other gasification schemes. The carbon rich char is then treated with steam in the gasification section to produce raw syngas while the heat for the reaction is provided by the hot flue gases of combustion flowing through the bayonet heat exchangers installed inside the gasifier reactor. Heating value of coal is fully utilized by downstream combustion of unreacted char in excess air.

Aspen Plus™ is used to simulate the process scheme for gasifier using a series of RCSTR reactors and the heat integration scheme (including coal precombustion, secondary gaseous combustor, and the combustion chamber for unreacted char downstream the gasifier). The heat transfer in the bayonet heat exchanger is simulated using the classical heat transfer correlations formulated in MS Excel™. The gasifier model, the heat integration scheme, and the heat transfer in the bayonet exchanger are iteratively converged to obtain final results. Comparison of the results generated by this simulation is made with published performance attributes of existing plants.

2. Process Description

The overall process scheme is shown in Figure 1.

Coal is introduced in the coal precombustion chamber at the reactor top where it is dried, pyrolyzed and partially oxidized with controlled amount of preheated air injected in the bottom at 550 °C and 1 barg pressure. According to Ma et al. (1989), for sub-bituminous coals, 50-70 % of sulphur converted in a typical gasification reaction is released during pyrolysis. In the precombustion section, the remaining sulphur is converted to hydrogen sulphide in the presence of high temperature and insufficient oxygen, thus leading to minimal production of sulphur oxides. The carbon monoxide rich gases generated in precombustion section carry along the moisture and the volatile matter of coal. This stage removes the tars and sulphur from the coal thus preparing a cleaner feedstock for the actual gasification process. The desulfurization of this gas stream can be simply carried out using dry desulfurization systems or the more common and widely used iron sponge process on a much reduced volume of gas to be handled as compared to conventional procedures, where the entire syngas from the gasifier needs to be cleaned using a series of columns for sulphur compounds removal. After H_2S removal, the CO-rich gases (containing volatiles and moisture) flow to the gas burner where they are further oxidized to sustain the endothermic gasification process. These flue gases are passed through bayonet heat exchangers vertically installed inside the gasifier for the transfer of heat to the steam and coal mixture in the moving bed around the bayonets. Eventually, at the exit from bayonets after providing heat for gasification, the still-hot flue gases are utilized for air preheat and vaporization of feed water to be introduced in the steam jacket of gas burner.

The char and ash mixture from the precombustion section flows down to the gasifier. The superheated steam is injected in the gasifier bottom at 900 °C temperature and 34 barg pressure. Raw syngas is taken at the gasifier top. The unreacted char with ash is fed into a combustion chamber downstream the gasifier. The hot air stream needed to completely burn the ash/unreacted char mixture is well in excess and is then used in the gas burner for CO rich gases as mentioned above. To maintain the temperature of flue gases at 1300 °C, high pressure steam is generated in the steam jacket of the gas burner vessel which is a part of the thermal integration of the process. The steam generated in the jacket is much in excess to the process requirement and thus provides a possibility of surplus steam for power generation.

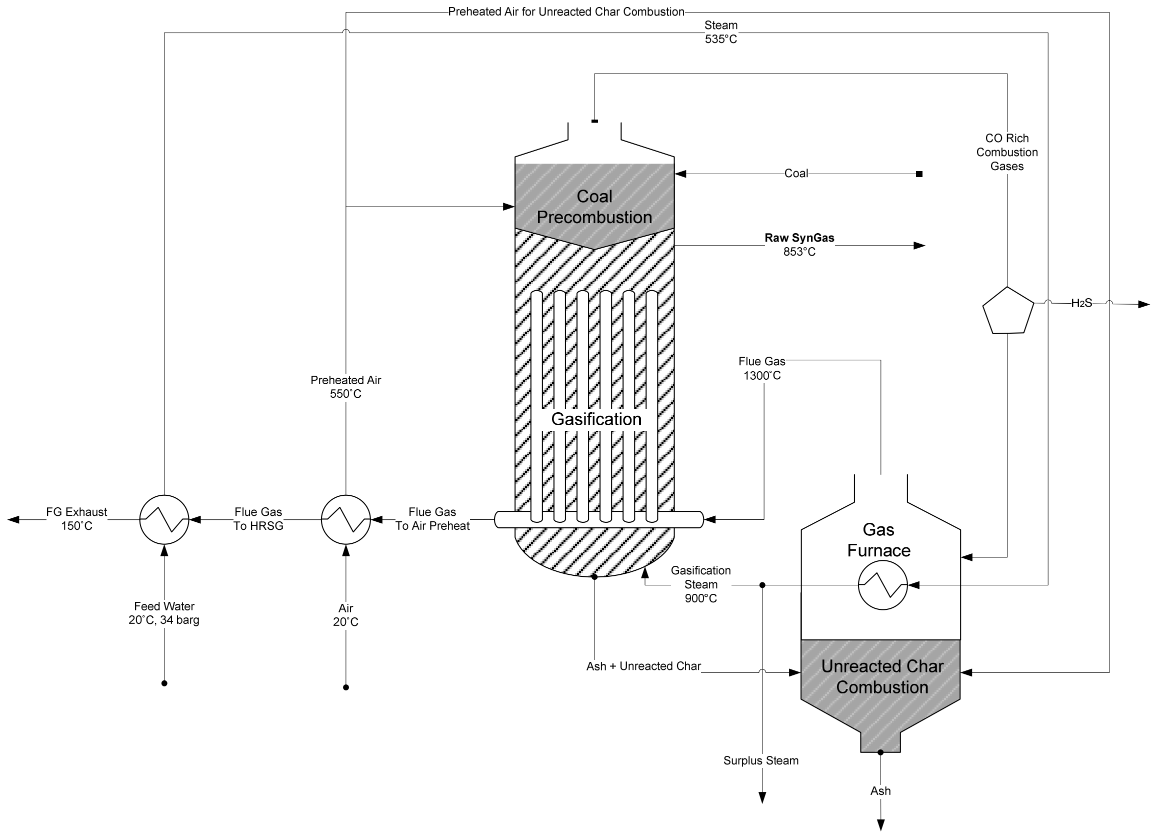

Figure 1: Schematic of the steam gasification of coal with precombustion.

3. Simulation Development

3.1 Gasifier

To simulate the gasifier, several modifications were made in the oxygen-steam simulation provided by Aspen Plus™ (2010) to cater for the proposed process. The property calculation method was changed to RK-BM. The gasifier is modelled by a series of 12 equal volume RCSTR blocks with a larger volume RCSTR block both at the beginning and at the end of the series to represent the adiabatic sections in the gasifier above and below the bayonet tubes. The pressure of each block is 34 barg.

3.2 Bayonets

The heat transfer model for the bayonet heat exchanger is based on the one developed by Bussman et al. (2005) for variable test furnace cooling in process industries. The model is modified for the vertical installation, axial flow regime of gases outside the bayonets, and reversed direction of heat transfer for the proposed scheme. The model is developed in MS-Excel™ with the temperatures and fluid properties imported from Aspen Plus™.

Hot Flue gases from the furnace enter the inner tube of the bayonet and rise to the end of the inner section. At this point, they turn back, and enter the annular section of the bayonet tube, flow back downwards and then discharge from the tube to the circuit downstream. The inner tube material is considered to be sintered α-SiC ceramic material to withstand the flue gases entering the bayonet tubes at 1300 °C (Munro, 1997), while the annular section is considered to be made of HK-40 heat resistant alloy (NiPERA, 1974) for efficient heat transfer to the mixture of steam & raw syngas in the reactor environment around these bayonet tubes.

The height of each bayonet tube is 18 m to allow the required heat transfer to the gasification reaction. To facilitate the calculations and profiling of the heat transfer and temperature distribution along the length of the bayonet tubes, these are divided in 12 hypothetical cells of length 1.50 m each corresponding to 12 RCSTR blocks for the gasifier simulation. Figure 2 shows the construction of a bayonet tube considered along with the temperature profile inside the bayonet centre pipe, bayonet annulus section and the gasification temperature from top to bottom of the bayonet length.

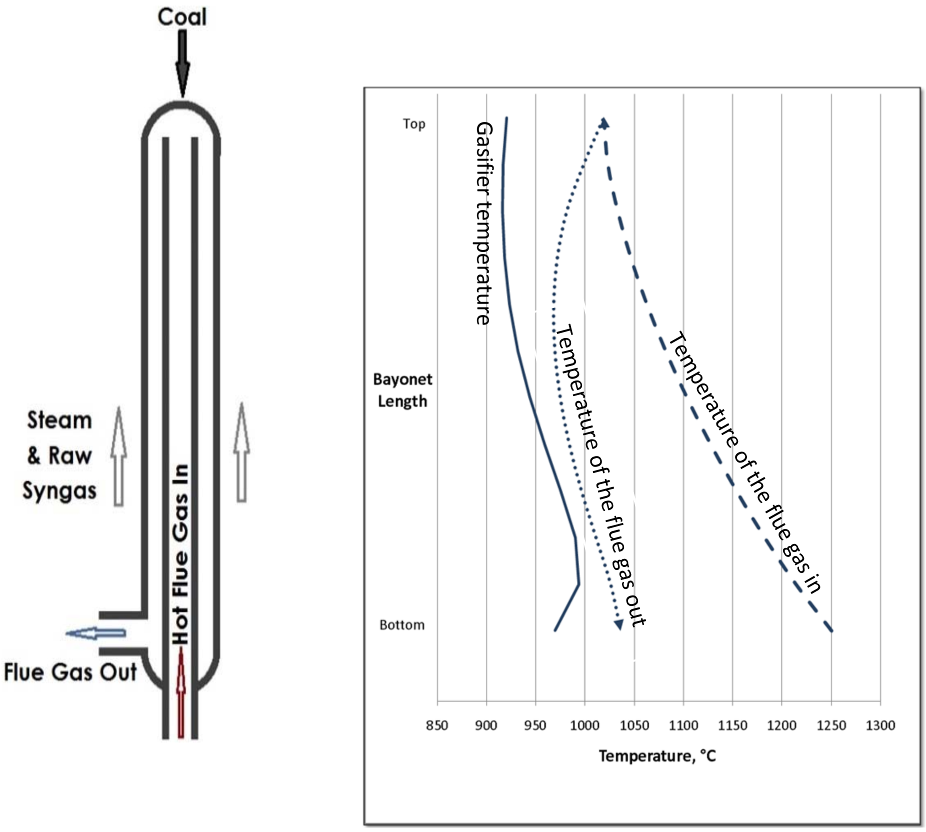

Figure 2: Construction of a bayonet tube heat exchanger and the temperature profile in various sections.

3.3 Hydrogen Sulfide Removal

H_2S removal from the fuel gas stream is modeled as an ideal separation block. A number of H_2S removal schemes have been developed which can reduce H_2S levels as low as 1 ppm as reported by Magomnang and Villanueva (2014).

3.4 Input Parameters

Table 1 summarizes the geometry of the gasifier and the bayonet tubes considered on the basis of industrial plants' configurations. Table 2 represents the feedstock conditions for the gasifier simulation.

Table 1: Geometric characteristics of the gasifier and bayonets

Reactor Vessel		**Bayonets**	
Parameter	**Value**	**Parameter**	**Value**
Height	28.0 m	Height	18.0 m
Diameter	5.0 m	Number of bayonet tubes	487
Adiabatic sections' height	5.0 m	Number of tube banks	15
		External tube outer radius	5.0 cm
		Internal tube outer radius	3.8 cm
		Tubes' thickness	0.5 cm
		Distance between two consecutive bayonets in a tube bank	1.0 cm
		Distance between two consecutive tube banks	22.0 cm
		Minimum Clearance between wall and the tube banks	22.0 cm

Table 2: Input parameters of the coal used in the proposed model (Aspen Plus, 2012)

Coal		**Proximate Analysis**		**Ultimate Analysis**		**Sulphur Analysis**	
Seam	Pittsburgh # 8	**Component**	**wt. %**	**Component**	**wt. %**	**Component**	**wt. %**
Feed rate	50,000 kg/h	Moisture	04.58	C	77.76	Pyritic	0.87
Particle size	1.0 cm	Fixed Carbon	37.37	H	05.24	Sulfate	0.87
Coal-to-steam ratio	0.5	Volatiles	50.31	N	01.47	Organic	0.88
		Ash	07.74	S	02.62		
				O	04.79		
				Ash	08.12		

Table 3: Simulation results compared to conventional gasification processes with Pittsburgh seam coal

Process	**This Scheme**	**Lurgi Gasifier**	**GE Gas Air**	**Babcock - Wilcox**
Mole % Composition (dry basis)				
CO	24.91 %	16.9 %	23.8 %	55.5 %
H_2	55.43 %	39.4 %	17.0 %	28.3 %
CO_2	17.46 %	31.5 %	6.7 %	6.93 %
CH_4	2.21 %	9.0 %	3.2 %	-
N_2	-	1.6 %	49.2 %	0.88 %
H_2S, Tars and other compounds	-	1.6 %	0.1 %	8.39 %
Condensate/Dry Syngas, (kg/kg)	0.59	1.97	0.21	0.16
% Conversion of C	93.77 %	90.6 %	88.5 %	99.0 %
H_2/CO Molar Ratio	2.23	2.33	0.71	0.51
Dry gas yield, Nm^3/kg coal	2.40	2.10	3.35	2.11
Cold Gas Efficiency, %	69.57 %	75.3 %	75.8 %	77.0 %
HP Steam in surplus(+)/required(-), kg/kg coal	+1.93	-2.59	-0.45	-0.20
Oxygen required, kg/kg coal	-	0.63	-	0.991
Power Generated(+)/Consumed(-), Watt/kg coal	+640	-252	-	-396

4. Results and Discussion

Simulations of the proposed gasification scheme with precombustion of coal feedstock are performed using Aspen Plus™ for the gasifier modelling and for heat integration modelling and using MS-Excel™ for the calculation of the heat transfer through the bayonet tube heat exchangers to the gasifier. All three schemes were iteratively run until they were simultaneously converged. Table 3 shows a summary of the product attributes from the simulation of the proposed scheme compared to those from the gasification of coal feed from Pittsburgh seam in the conventional gasification processes as reported by Wen et al. (1975) and Furusawa et al. (1985).

The molar composition of the dry syngas produced in the proposed scheme has a lower amount of CO_2 as compared to the most widely used Lurgi gasifier. Though the CO_2 composition is even lower in the GE and the Babcock-Wilcox processes, yet it is overshadowed by the lean product gas due to nitrogen and high requirement of power for oxygen production per kg of coal, respectively. The product gas contains less contaminants as compared to other schemes.

This scheme has an adequate conversion of carbon because the unconverted carbon is combusted downstream for the process heat generation leading to the generation of surplus steam and consequent generation of power apart from syngas. In other configurations there is a higher power input of electrical energy required per kg of coal to produce pure oxygen, around 46 MJ_e/kmol O_2 (Higman and Burgt, 2007).

Among the oxy-steam gasification processes listed above, the proposed scheme shows an appropriate molar ratio of hydrogen and carbon monoxide making the product suitable for downstream processes. Compared to other processes, the cold gas efficiency of the presently proposed scheme seems less but it should be taken into account that the process is not only energetically self-sufficient but produces surplus steam convertible to power. The effective efficiency of a conventional gasifier such as Lurgi process goes down from 75.3 % to 48.8 %, considering the amount of coal needed to generate energy for the production of steam and power required for the process (Wen et al, 1975).

5. Conclusions

In this work, an indirect gasification process has been developed and discussed with the precombustion of coal and the heat for gasification supplied through bayonet tube heat exchangers installed inside the gasifier. The gases produced in the precombustion of coal take away tars and volatiles including hydrogen sulphide leaving cleaner char ready for gasification. These gases can be cleaned before complete combustion downstream. The char is gasified with high pressure and high temperature steam while the heat for the process is provided using bayonet tube heat exchangers. The process results to be fully heat integrated and energetically self-sufficient.
The process cold gas efficiency is comparable to other gasification processes using similar coal keeping in view that external energy is required for the utilities (steam and power) in conventional processes, while in this model surplus steam is generated at high pressure for power generation apart from the syngas produced.

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