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Simulation and Sensitivity Analysis for H_2 Production Using Steam Oxygen Gasification in Aspen Plus

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ABSTRACT

In this study, steady state simulation model of steam oxygen gasification has been developed in Aspen Plus for hydrogen production using Pakistani Thar coal. Aspen Plus is selected as a simulation tool due to its higher capability of handling solid feed using physical models. Steam oxygen gasifier has been modeled in two steps; first utilizing DECOMP succeeding RGibbs unit operation model. Simulation results include; sensitivity analysis of coal slurry concentration , oxygen to coal mass ratio and gasifier operating temperature. Influence of the above mentioned parameters are analyzed on lower heating value of syngas, thermal efficiency, gasifier efficiency and molar fraction of hydrogen in enriched syngas.Simulation results provide the following optimal operating conditions; 50% solid concentration, 0.48 O_2 to coal mass ratio, low shift reactor operating temperature 473 K, high shift reactor operating temperature 623 K and gasifier operating temperature 1173 K for the production of syngas having 92% H_2 molar composition.

1. Introduction

In spite of expeditious advancement and introduction of alternative and renewable energy resources, coal still keeps on being the most noteworthy fuel to fulfill worldwide power demand. Everywhere throughout the world, many countries are getting energy from lignite coal. Pakistan is utilizing negligible fraction of coal as compared to other countries in the world as depicted in Table 1 [1, 2]. Coal is more useful for power production from an economical point of view as it is readily available in Pakistan and can be easily transported and stored while going over an extensive distance [3, 4].

Pakistan has considerable coal reserves. However; its significant amount is low quality lignite coal. Suitable technology should be explored to extract energy from low-quality lignite coal for better plant operation and easy maintenance [4].

Steam oxygen gasification is especially used for this purpose as it can be utilized for electricity production. For the simulation of steam oxygen gasification process, Aspen Plus software is chosen because of its significant worth to simulate various chemical processes particularly biomass gasification and petroleum industry as it has ability to handle solid carbonaceous feed to model steady state processes.

The aim of this study was to analyze and simulate steam oxygen gasification process and onward processing for hydrogen enriched syngas. Thar coal was taken as feed as its coal reserves in Pakistan are approximately 175,506 million tons [4, 5].

2. Process Description

Gasification is the main step in steam oxygen gasification (SOG) process and all the SOG power plants follow the same processing steps except carbon dioxide sequestration (CCS). The main steps in SOG process are [6]:

i. Air separation unit (ASU) produces pure oxygen and nitrogen. Pure oxygen is used in gasification and pure nitrogen for gas dilution, sweep and as a carrier source.
ii. Coal particles are crushed into small particlesand transferred by pneumatic conveyor in the form of slurry or as dry feed.
iii. Mainly gasification occurs three steps;; oxidation, pyrolysis and gasification.
iv. In water gas shift (WGS) reaction to convert approximately all CO convert into CO_2 and production of H_2.
v. Finally, capture of all these impurities (NH_3, COS, H_2S , chlorides and fluorides) from syngas to produce H_2 enriched syngas during gas purification processing.

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Table 1: Review of worldwide electricity generation from different resources

Resource	World	Pakistan	Australia	China	Germany	India	USA
Coal	40.8%	0.1%	76.8%	79.1%	45.6%	68.6%	48.8%
Oil	5.5%	35.4%	1.1%	0.7%	1.5%	4.1%	1.3%
Gas	21.2%	32.4%	15.0%	0.9%	13.8%	9.9%	20.8%
Nuclear	13.5%	1.8%	0.0%	2.0%	23.3%	1.8%	19.2%
Hydro	16.2%	30.3%	4.7%	16.9%	4.2%	13.8%	6.5%
Other	2.8%	0.0%	2.5%	0.5%	11.6%	1.9%	3.4%
Total	100.0%	100.0%	100.0%	100.0%	100.0%	100.0%	100.0%

As described earlier in first step coal lumps are crushed into small particles; approximately 100μm and directed to fixed bed gasifier. Steam and oxygen are used in gasifier as oxidizing agents and various reactions takes place as written below [7, 8, 9].

Carbon Reactions

$$C + CO_2 \rightarrow 2CO \quad 172KJ/mol \quad (1)$$

$$C + H_2O \leftrightarrow CO + H_2 \quad 131KJ/mol \quad (2)$$

$$C + 2H_2 \leftrightarrow CH_4 \quad -74.8KJ/mol \quad (3)$$

$$C + 0.5O_2 \rightarrow CO \quad 111KJ/mol \quad (4)$$

Oxidation Reactions

$$C + O_2 \rightarrow CO_2 \quad -394KJ/mol \quad (5)$$

$$CO + 0.5O_2 \rightarrow CO_2 \quad -284KJ/mol \quad (6)$$

$$CH_4 + 2O_2 \leftrightarrow CO_2 + 2H_2O \quad -803KJ/mol \quad (7)$$

Methanation Reactions

$$2CO + 2H_2 \rightarrow CH_4 + CO_2 \quad -247KJ/mol \quad (8)$$

$$CO + 3H_2 \leftrightarrow CH_4 + H_2O \quad -206KJ/mol \quad (9)$$

$$CO_2 + 4H_2 \rightarrow CH_4 + 2H_2 \quad -165KJ/mol \quad (10)$$

After production of syngas in the gasifier, it enters into water gas shift reactor where approximately all CO is converted to CO_2 and hydrogen.WGS reaction occurs in two stages in the presence of catalyst; high temperature and low temperature shift reaction subsequently [2]. Catalyst used in HTS is a mixture of 0.2% MgO, 10% Cr_2O_3, 74.2% Fe_2O_3 and remaining would be volatiles. While catalyst used in LTS is a mixture of 15-20% CuO, 68-73% ZnO, 2-5% Mg, Al and Mn oxides, 15-33% Al_2O_3, 34-53% ZnO, and 32-33% CuO [10,11].

For the removal of impurities (NH_3, COS, H_2S and CO_2), gas is passed through a absorption column where various physical or chemical solvents are used for absorption. In this study, methanol is used as a solvent for physical absorption of gases as it has the tendency to co-capture CO_2 and H_2S as well as COS. This co-capturing process has significant benefits both economically and technically over H_2S and CO_2 capture individually [7]. After CO_2 capture, plant electrical output decreases approximatley by 8% [11].

Produced hydrogen enriched syngas can be further used for various applications; in combustion to run the gas turbine, in Integrated Gasification Combined Cycle (IGCC), as a purified fuel etc. Complete block flow diagram has been shown in Fig. 1 [11].

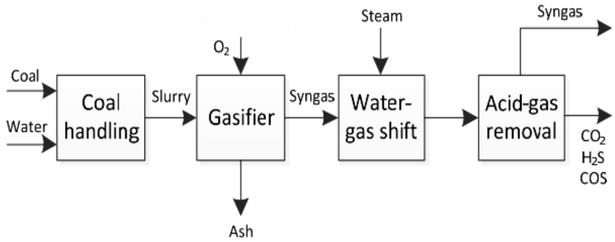

Fig.1: Simplified block flow diagram for hydrogen production

3. Aspen Plus Model Development

3.1 *Physical Property Method*

Definitions of species are specified to simulate a model in Aspen Plus. The utmost significant species in coal gasification are; O_2, C, CO_2, CO, H_2, H_2S, CH_4, N_2, HCN, HCl, NH_3, S, SO_2 and COS. While CS_2, metals (Se and Hg), Mercaptans and alkali components are neglected as these are present in trace amounts and if considered, decrease the convergence performance of the model. Redlich-Kwong-Soave Method is used as global subsystems. STMNBS and nonrandom two liquid-Redlich Kwong (NRTL-RK) property methods are used where whole or even partially, water is present [11]. The HCOALGEN and DCOALIGT models are utilized to calculate enthalpy and density for ash and coal. In Aspen Plus, different unit operation models are used to simulate steam oxygen gasification process for the production of hydrogen enriched syngas (Table 2).

3.2 *Methodology and Model Assumptions*

Following parameters are considered as assumptions to develop this simulation model; (i) Steady state process; (ii) heat losses are neglected; (iii) all equipments are considered insulated; (iv) feed rate of coal 3.472 kg/sec; (v) 98% purified oxygen is used as an oxidizing agent; (vi) coal tar is not considered in this model. In this

Table 2: Detail of Aspen Plus models used in model development

Unit operation	Aspen Plus model	Specification
Coal crushing	Crusher	Rigorous simulation of particles size distribution
Coal particles screening	Screen	Rigorous simulation of the separation efficiency of the screen
Coal gasification	Equilibrium Reactor based on Gibbs energy minimization (RGibbs)	Specification of the possible products: CH_4, HCN, H_2O, O_2, H_2 , Cl_2, HCl, CO, CO_2, C, COS, H_2S, NO, NO_2, N_2, NH_3, SO_2, S, SO_3
Dust removing	Separation (SEP)	Simplified simulation of gas/solid separation by fixed split fraction specification together with the temperature drop
HTS Reactor	Equilibrium Reactor based on stoichiometric calculation (REquil)	Specify Stoichometric Reactions. OT 624 K, OP 3.9 Mpa
LTS Reactor	REquil	Specify Stoichometric Reactions OT 474 K, OP 0.6 Mpa
CH_3OH	Rigorous Fractionation (RadFrac)	Removal of SO_2, H_2S, HCN, NH_3, COS Top stage pressure 3.3 MPa, SN 10

model, gasifier has been modeled into two steps. RYield model is used to break large chain coal molecules into smaller elements. After it, RGibbs reactor is used to model next step of gasification and specify the expected products which will produce in syngas.

After gasification, syngas enters into water gas shift reactor where almost complete CO converts into $H_2$and CO_2. To enrich H_2 concentration in syngas, different impurities like CO_2, H_2S, COS and NH_3 are removed from syngas by using methanol solvent [10, 11]. Composition of Thar coal is written in Table 3 [13, 14, 15]. Complete process simulation model diagram has been depicted in Fig. 2 & Fig. 3.

Table 3: Thar coal analysis

Analysis	(%)
Proximate analysis (dry basis)	
Ash (%)	19.37
Volatile Matter (%)	48.52
Fixed Carbon (%)	23.66
Moisture (%)	8.50
Ultimate analysis	
Ash (%)	19.37
Hydrogen (%)	2.94
Carbon (%)	49.93
Nitrogen (%)	00.98
Sulphur (%)	4.02
Oxygen (%)	14.26
Cl_2 (%)	8.50
Heating Value (Btu/lb)	6,244-11,045

3.3 Model Validation

Results of Aspen Plus process simulation model developed in this study is validated with results from published literature [9]. In the present study, fixed bed gasifier has been modeled and Thar lignite coal is taken as feed while in the reference article, entrained flow gasifier has been modeled and Colombian bituminous coal is used as feed. The difference between these two gasifiers is that entrained flow gasifier operates at high temperature and pressure having high demand of oxidant while fixed bed gasifier operates at low temperature with low demand of oxidant. In entrained flow gasifier, ash is removed as molten slag while in fixed bed gasifier; ash is removed as dry or ash. Coal particle size below 0.1mm is required in entrained flow gasifier. On the other hand, particle size of the range 6 to 50mm is entered in fixed bed gasifier [9]. Moreover, sensitivity analysis of high temperature shift (HTS) reactor operating temperature and gasifier operating temperature are also studied in the present study which did not reported in literature.

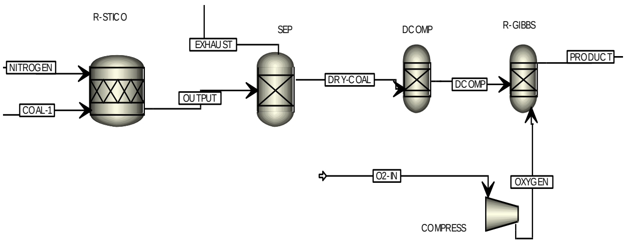

Fig. 2: Aspen Plus flow sheet model for fixed bed gasifier

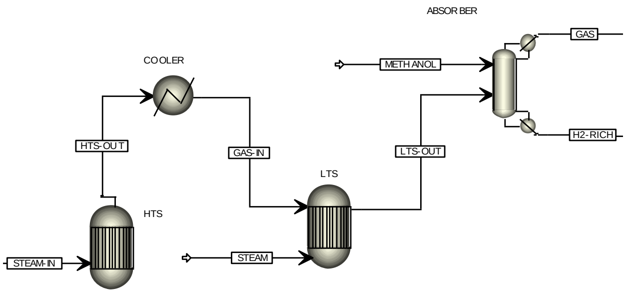

Fig. 3: Aspen Plus flow sheet model for production of H_2-enriched syngas from gasifier exhaust gas stream

4. Results and Discussion

Sensitivity analysis is advantageous to obtain best operating condition for a process which will be beneficial to improve the performance and efficiency of the system. Following variables are chosen in sensitivity analysis (i) Gasifier operating temperature; (ii) Mass solid concentration in coal slurry; (iii) High temperature shift (HTS) reactor operating temperature; (iv) Low temperature shift (LTS) reactor operating temperature; (v) O_2 to coal mass ratio. In Sensitivity analysis, impact of selected variables are studied on the following parameters (i) Thermal efficiency; (ii) Lower heating value; (iii) Overall CO conversion in water gas shift reactor; (iv) H_2 molar fraction in rich syngas; (v) Gasifier efficiency; (vi) Massflow rate of different components in gas stream leaving the gasifier. Gasifier and thermal efficiencies are described as below:

4.1 Gasifier Efficiency

The gasifier efficiency is defined in Equation 1[11].

$$\eta_{gasifier} = \frac{LHV_{sg}.Q_{sg}}{LHV_f.R_f} \quad (1)$$

Where $\eta_{gasifier}$ is the cold gas efficiency of gasification (%); Q_{sg} is the volumetric flow rate of syngas (m^3/s); R_f is the gasifier coal consumption rate; LHV_f is the lower heating value of the coal input (kJ/kg) and LHV_{sg} is the lower heating value of the syngas (kJ/m^3) [11].

4.2 Thermal Efficiency

The thermal efficiency is defined in Equation 2 [5]

$$\eta_{Th}(\%) = \frac{M_{syn} \times LHV_{syn}}{(M_{Coal} \times LHV_{Coal} + Q_{Aux})} \times 100 \quad (2)$$

Here M_{syn} and M_{Coal} are the mass flow rates of syngas and coal respectively; LHV_{syn} and LHV_{coal} are the lower heating values of syngas and coal respectively [4]; Q_{Aux} is the power required for auxiliary functions. LHV_{syn} (kJ/Nm^3) can be calculated from Equation 3[5];

$$LHV = (119950.4 \times n_{H_2} + 10103.9 \times n_{CO} + 50009.3 \times nCH4 \times \rho \quad (3)$$

Gasifier and thermal efficiency directly represent process performance. LHV_{syn}, thermal efficiency and H_2 molar fraction have been shown against sensitivity analysis variables (Table 4 & 5). O_2 to coal mass ratio has a significant impact on the thermal efficiency and H_2 molar fraction as shown in Table 4. Gasification reaction rate increases as O_2 to coal mass ratio increases. It will increase up to specific limit of O_2 to coal mass ratio. Onwards this specific limit of O_2 to coal mass ratio, gasification reaction will move towards complete combustion reaction. In Fig. 4, it can be seen that O_2 to coal ratio has almost negligible impact on overall CO conversion in WGS reaction while maintaining constant HTS and LTS temperature. On the other hand, H_2 molar flow increases continuously in leaving stream from shift gas reactor as O_2 to coal ratio has large impact on the reaction rate occurring in gasifier.

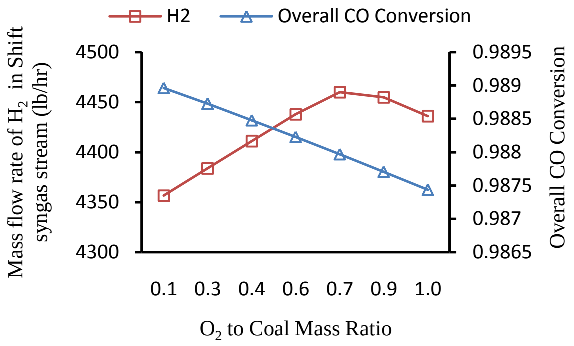

Fig. 4: H_2 mass flow rate and CO conversion verses O_2 to coal mass ratio.

Coal slurry concentration has less impact on LHV_{syn} and H_2 molar fraction as compared to O_2 to coal ratio. Coal slurry concentration has direct relation to thermal efficiency while it is inversely related to H_2 molar fraction as shown in Table 4

On the other hand, coal slurry concentration has very small impact on LHV_{syn}. As coal slurry concentration increases, temperature will rise in gasifier and more CO will be produced in the gasifier but overall final CO conversion will be restricted due to steam flow rate entering the WGS reactor. Up to 48% of solid concentration, H_2 concentration will increase in syngas. Onward, it starts to decrease due to limited availability of steam in WGS reactor. WGS reaction occurs in two stages high temperature and low temperature respectively. Variation in HTS reactor operating temperature does not have a noteworthy impact on LHV_{syn}, H_2 molar concentration and thermal efficiency as depicted in Table 4.

While LTS temperature has significant impact on H_2 molar concentration and thermal efficiency as shown in Table 4. WGS reaction is an exothermic reaction and CO conversion is favorable at low operating temperature in reactor. In Fig. 5, H_2 molar concentration decreases with

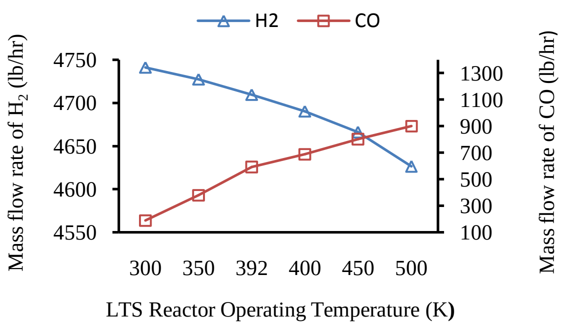

Fig. 5: Mass flow rate verses LTS reactor operating temperature

Table 4: Study effect of various parameters on LHV, H_2 molar fraction and thermal efficiency

Parameter	LHV (MJ/m^{-3})		H_2 molar fraction enriched syngas		Thermal efficiency (%)	
	Calculated	Literature	Calculated	Literature	Calculated	Literature
O_2 to Carbon mass ratio						
0.16	15.19	20.9	0.87	0.561	47.3	34.1
0.32	16.72	15.1	0.91	0.806	47.8	42.2
0.48	17.26	13.0	0.96	0.895	50.0	52.0
0.64	14.77	12.0	0.89	0.922	45.5	62.6
0.8	13.02	10.8	0.84	0.977	32.8	60.1
0.96	10.97	10.7	0.71	0.983	30.4	54.5
Coal slurry concentration (%)						
86.21	9.01	10.8	0.87	0.926	57.09	61.3
75.47	9.06	10.8	0.89	0.971	56.63	60.4
65.01	8.90	10.8	0.87	0.979	54.00	59.9
56.34	8.50	11.0	0.91	0.974	53.20	59.2
50	8.10	11.5	0.93	0.958	51.27	58.4
LTS reactor operating temperature (K)						
453	9.05	10.7	0.93	0.983	51.50	59.5
473	9.45	10.8	0.91	0.979	52.51	59.9
498	9.41	10.8	0.89	0.971	54.63	60.4
523	9.32	10.8	0.88	0.962	55.65	61.5

increase in LTS reactor operating temperature while CO molar concentration increases. Therefore at higher operating temperature in LTS, less acid gas will be present in the downstream of WGS and less solvent will be required for its removal as well as lowers the energy requirement will be for regeneration of solvent. This is the reason that thermal efficiency increases at higher operating temperature in LTS.

Table 5: Analyze effect of various parameters on LHV, H_2 molar fraction and thermal efficiency

Parameter	LHV (MJ/m^{-3})	H_2 molar fraction in enrich syngas	Thermal efficiency (%)
HTS reactor operating temperature (K)			
600	15.65	0.97	51.50
640	12.53	0.97	51.22
680	10.96	0.96	51.03
720	9.39	0.96	50.50
Gasifier operating temperature (K)			
923	12.82	0.78	49.15
973	12.89	0.89	51.15
1023	13.05	0.91	52.54
1073	13.90	0.94	54.55
1123	14.90	0.98	55.89
1173	15.50	0.98	56.52
1223	16.45	0.96	53.37
1273	17.04	0.93	50.15

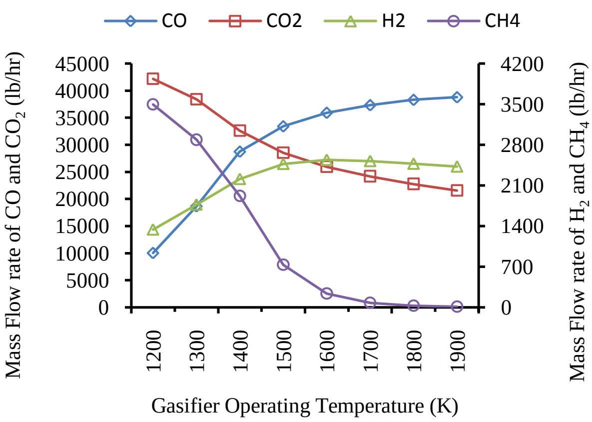

Fig. 6: Mass flow rate verses gasifier operating temperature

5. Summary

Gasifier temperature has a large impact on LHV_{syn}, thermal efficiency and hydrogen molar concentration. H_2 molar fraction and thermal efficiency increase up to certain limit of gasifier operating temperature in the range of 923 K to 1173 K (Table 5). Furthermore, its starts to decrease because more by-products are produced as compared to H_2 production rate as shown in Fig. 6.

On the other hand, gasifier efficiency which represents carbon conversion to desired products increases with an increase in temperature up to 1173 K after it tends to decrease. Thermal efficiency trend has been shown in Fig. 7.

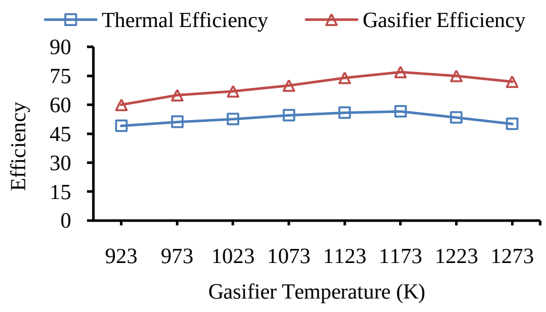

Fig. 7: Gasifier and thermal efficiency verses gasifier temperature

Finally in this study, SOG process is simulated and sensitivity analysis has been performed. The impact of different variables on LHV_{syn}, thermal efficiency and H_2 molar fraction in H_2 enriched syngas was observed. It is also clearly perceived that HTS operating temperature has no significant impact on LHV_{syn}, thermal efficiency and H_2 molar fraction. Gasifier operating temperature has a convincing impact on H_2 molar fraction (0.98) and thermal efficiency 56%. O_2 to coal mass ratio, coal slurry concentration, gasifier and LTS reactor operating temperature has more prominent effect on thermal efficiency while HTS reactor operating temperature has negligible impact on thermal efficiency.

In this process simulation model, main equipment is gasifier where maximum conversion of carbon to desired products attains. Optimal operating conditions and parameters for H_2 enriched syngas are 50% solid concentration, 0.48 O_2 to coal mass ratio, LTS reactor operating temperature 473 K, HTS reactor operating temperature 623 K and gasifier operating temperature 1173 K.

6. Conclusions

At these optimum conditions, the final H_2 enriched syngas composition is given in Table 6. From literature, it is found that 90% or above H_2 enriched syngas is suitable for combustion to run gas turbine and also for fuel purposes [16, 17].

Table 6: Molar fraction of H_2-enriched syngas

Component	Molar fraction
H_2	0.92
N_2	5.35×10^{-03}
H_2O	1.89×10^{-48}
Cl_2	1.06×10^{-12}
CO	4.70×10^{-3}
CO_2	5.80×10^{-2}
CH_4	1.50×10^{-2}
H_2S	6.56×10^{-6}
COS	2.47×10^{-7}
NH_3	2.19×10^{-16}
CH_3OH	3.00×10^{-4}

Hence, it is concluded that Pakistani Thar coal is suitable for gasification. It can be used either in IGCC power plant or for H_2 fuel production. This study was an initial step to check the feasibility of Thar coal for gasification. Further performance can be improved by heat integration and using more advanced technology of coal gasification.

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