

Aspen Plus® Simulation of a Coal Gasification Process (Geometric Analysis)

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Abstract

A semi-batch foam-flotation in which air is continuously sparged through an emulsion, with added surfactant, a coagulant, and a solvent, has been shown to be effective in the treatment of steel-rolling mill effluents. The effect of time of flotation, effects of surfactant and alum concentrations, and effect of the solvent volume were all experimentally explored. The oil recovery increased with concentrations of alum and sodium lauryl sulphate of up to around 4 g/l, and then leveled off. Volume of the solvent layer at the top improved the separation of oil with an optimum ratio of 0.167 ml solvent per ml of emulsion. The oil separation was highest for the time of flotation of about 25 minutes, and re-emulsification of the separated self-emulsifiable oil was observed beyond this time. A model reported in the literature for the semi-batch flotation has been shown to be inadequate in predicting the experimental data on separation of oil. A mathematical model developed for the separation by foam flotation based on an analogy with a chemical reaction was found to be appreciably better in its predictive capability than the one reported in literature. The new mathematical model has established the separation of oil by foam flotation as a second-order process, and its predictions can be further fine tuned using a parameter referred to as a sticking coefficient (β). The values of β for the two effluents investigated were equal to 7.9×10^{-5} and 6.7×10^{-5} , respectively.

Keywords: Aspen plus simulation; Bayonet heat exchanger; Coal gasification; Moving bed gasifier; Syngas

Introduction

Energy demand increases day by day at National and International level. The energy system was not attuned to technology which determined the demand and supply equation. Currently, the major challenge is that petroleum and natural gas reserves have been consumed so rapidly along with continuously demand coming from technology emerging countries, their price is also increasing since many years affecting the global economy negatively [1].

Coal is currently a major energy source, with regard to contributing to the world's energy systems. Coal is indeed a potential threat to the environment because of products during the gasification process. The liquefaction and gasification of coal has gained attention for developing cleaner and environmentally safer fuels [2,3].

It is obvious that the world fossil fuel reserve, in which the whole world is dependent are not infinite, so it is the time to look for replacement. There were home-grown solutions available and coal above every other resource offered a natural option, but planners had been neglecting these for over three decades now. Pakistan is facing a serious issue of energy crises and has lagged behind in adopting modern technology to increase electricity production with lower fuel consumption. Hence increasing in the price of oil and diminishing natural gas reserves, forced to focus on coal fired plant to arrest rising power crises.

Behind the scene coal as a fuel added threat to the environment, because of having undesirable products that are produced during the combustion process. To have environmentally safer fuels, the liquefaction and gasification are under attention. The coal gasification is a process in which coal is partially oxidized to form the combustible gases which are carbon monoxide, hydrogen, and methane. The noncombustible products carbon dioxide and water are also formed. During the early 19th century and up until the 1940's, almost all fuel gas was produced by coal gasification. During the 1940's, natural gas became a cheaper alternative to gases derived from coal gasification. However, interest in coal gasification has been renewed due to depletion of natural gas reserves [4]. Gasification is an important route for

conversion of coal or solid waste materials to useful gaseous products for direct firing in thermal applications as well as for the production of liquid fuels or chemicals, and to reduce the environmental emissions as posed by the direct burning of coal [5]. In this study, Simulation of Coal Gasification process is performed using steam as the gasification medium rather than its mixture with pure oxygen as in current industrial practices. The purpose is to determine the performance of indirect gasification in order to make the process more economically and feasible by eliminating the costs of pure oxygen production.

The process consists of a gasifier and a furnace. Part of the syngas produced in the gasifier is combusted in the furnace to provide heat for the endothermic gasification process. The flue gases from the furnace pass through bayonet tubes to exchange heat within the coal bed in the gasifier. A model has been developed for the analysis of heat transfer among various regions of the bayonets and the gasifier environment.

The product gas, named Syngas obtained through gasification is a fuel source itself, and is generally a more efficient fuel than the initial fuel fed to the gasifier. Now this Syngas can either be burnt in Internal Combustion Engines (producing hydrogen and methanol) or alternatively used as a raw material for the Fisher-Tropsch process to convert into synthetic fuel [6].

Nomenclature

[CO]=Mean concentration of CO

[CO₂]=Mean concentration of CO₂

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T=Temperature, K

C_p = Specific heat of the flue gas, J/kg.K

k=Thermal conductivity of flue gases, W/m.K

μ =Dynamic Viscosity of flue gases, Pa.s

ρ_1 =Density of Inlet Flue Gases, kg/m³

qi=Heat provided for gasification by cell 'i' of a tube, W/tube

m=Mass flowrate of flue gases, kg/sec

LHV=Lower Heating Value

Process Model

The coal gasifier used in this simulation is a vertical reactor as shown in Figure 1, in which the coal is fed with the high pressure superheated steam and the heat for the endothermic gasification reaction is provided by the vertical bayonet tube heat exchangers placed in the reactor. The product gas from the gasifier is obtained from the reaction contains CO, H₂, CO₂, CH₄, and unreacted steam. The Ash is removed from the bottom of the gasifier along with unreacted carbon. Part of the syngas produced is burnt with air in a furnace to produce superheated steam and hot flue gases are then used to provide process heat through the bayonets.

In the topmost section of the gasifier, three adiabatic processes have been taken; coal drying, coal pyrolysis, and partial gasification of char. The heat for these processes has been taken from the hot gaseous mixture passing through the section until the point that all the material in the top section is in thermal equilibrium.

In the lower portion of the gasifier, the gaseous and solid reactants pass over the banks of bayonet tubes, which provide heat for the endothermic gasification process to continue until the desired conversion is achieved.

A heat exchanger bayonet is comprised of two concentric tubes, in which the fluid may flow in two different ways, as shown in Figure 2. The inlet can be through the center tube and the outlet from the outer annular section, or vice versa. The choice adopted depends on the type of process and operating conditions.

The advantage of this type of layout lies in the possibility of using high temperature heating streams provided that the bayonets are constructed with suitable materials that are resistant to high temperatures [7]. A further characteristic of this type of exchangers is the ability of the two concentric tubes to thermally expand independently from each other, thus making them suitable in environment with high temperature differences. This type of heat exchanger has already been employed in the "Topsoe Bayonet Reformer" for the production of syngas through the steam reforming of natural gas.

The purpose of this paper is to estimate the feasibility of using this exchanger in a gasification process indirectly. The possibility has been explored for the use of post-combustion flue gases as a thermal reactor, fed into the central portion of the bayonet tubes [8].

In the reactor, Coal is fed from the upper part while the steam is used as a gasifying medium entering the lower part. This forms a counter-current flow between the solid reactant and the gases. The moving bed type reactor is examined, in which the coal particles have a specific diameter. The hot flue gases flowing inside the bayonets are formed by the combustion of a part of the raw syngas produced in the gasifier furnace accordingly which shows into the process scheme of Figure 3.

Heat Integration

The heat required to provide various utilities for the gasification process to be carried on in the gasifier (steam and air for combustion) is taken mainly from the high temperature flue gases leaving from the furnace and from various process streams which need to be eventually cooled down; thus reducing the net amount of fuel required to be burnt in the furnace. The cooled syngas is divided into two parts. One part is drawn as the product stream for further processing and the other part is mixed with the preheated air to be fed in the furnace for the combustion process. The mixture of syngas and preheated air is then sent for combustion in furnace, where high temperature flue gases are generated. The saturated steam produced is then used for the generation of superheated steam using the heat from the high temperature flue gas from the furnace. The superheated steam thus produced is sent to the gasifier to take part in the gasification reaction. The flue gases from the gasifier bayonets are used to preheat the air requires for combustion in furnace. Continuous recovering of heat takes place to produce saturated steam for process utility.

Chemical Kinetics

In the process of char gasification, the following reactions are considered [9-11].

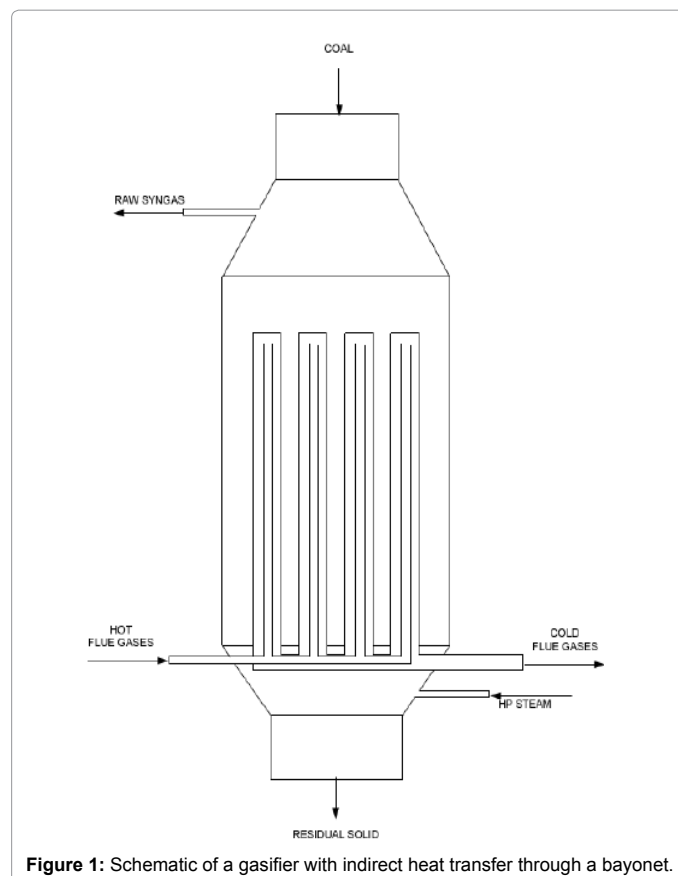
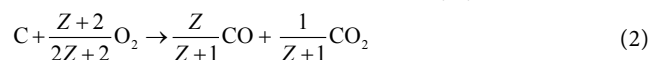
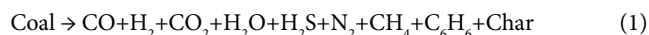


Figure 1: Schematic of a gasifier with indirect heat transfer through a bayonet.

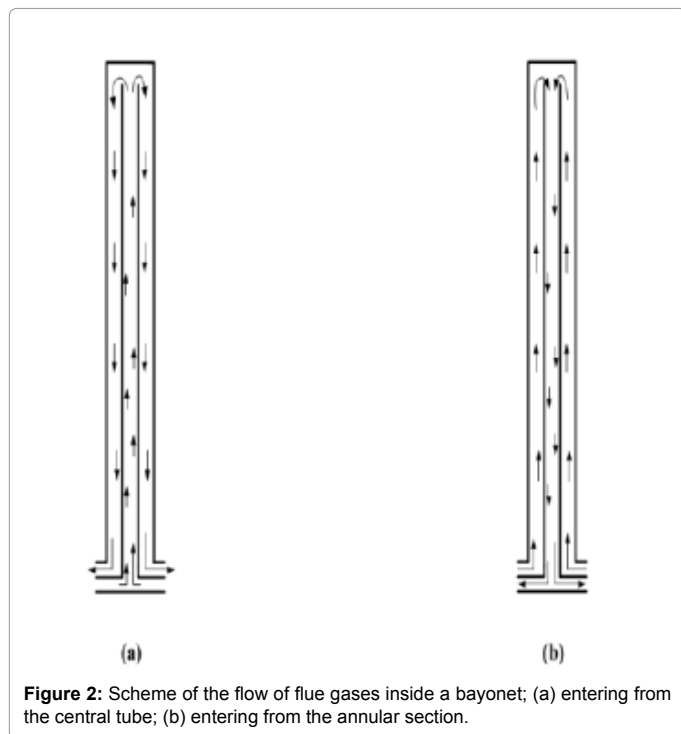


Figure 2: Scheme of the flow of flue gases inside a bayonet; (a) entering from the central tube; (b) entering from the annular section.

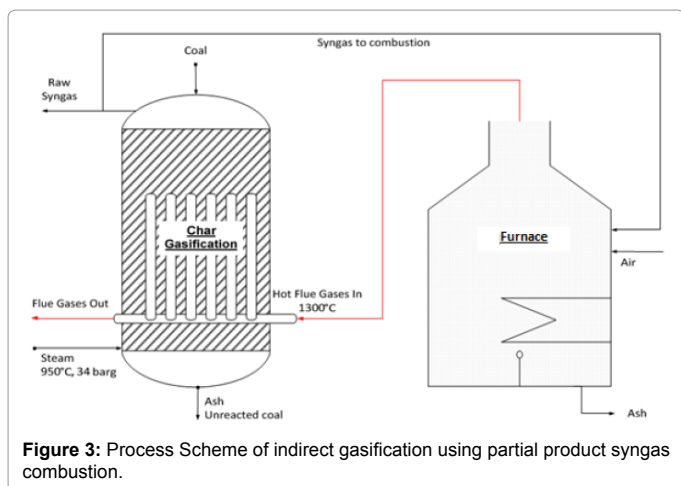


Figure 3: Process Scheme of indirect gasification using partial product syngas combustion.



$$Z = \frac{[CO]}{[CO_2]} = 2500e^{\frac{-6249}{T}} \quad (8)$$

Theoretical Model

This model is based on the one presented by Bussman et al. for cooling bayonets of testing burners in process industries. Bayonets are distinctive heat exchange devices comprising of two sections. Hot Flue gases from the furnace enter the inner tube of the bayonet and rise to the end of inner section. In this part, the flue gases lose enough heat to be able to come in contact with the outer section without damaging it. At the end of the inner tube, these gases turn 180 degrees and encounter

the annular section of the bayonet tube and flow back downwards and then discharge from the tube to the circuit downstream. These tubes are installed vertically on the reactor floor. To facilitate the calculations and profiling of the heat transfer and temperature distribution along the length of the tubes, these are distributed in 12 hypothetical cells [12,13].

Assumptions

Following assumptions were made while developing the model:

1. Thermal properties of the gas stream in each cell are at the mean temperature of each cell.
2. Radial heat transfer is dominant, so axial heat transfer can be neglected.
3. Flow of coal is the negative z-direction along the length of the tube heat exchanger.
4. Heat transfer by radiation is considered to take place from center pipe wall to the annulus inner wall and from annulus outer wall to the reactor volume.

Energy Balances

The energy balance were formed for each cell of the bayonet tube by taking into account the three modes of heat transfer i.e., conduction, convection and radiation. Following section were kept in consideration while performing energy balance in the gasifier, i.e., Bayonet center pipe inner wall, Bayonet center pipe outer wall annulus, Annulus inner wall, Annulus pipe outer wall and between two adjacent cells in the center pipe. Different heat transfer logics have also been used to analysis the flue gas temperature. The properties (C_p , μ , k , and ρ) of the flue gases passing through the bayonet tube heat exchangers and the those of the mixture of steam and syngas flowing over the outer surface of the bayonets are retrieved from the properties of streams and the individual gasifiers developed in the model for each scheme, where each reactor (GASF-1 to GASF-12) corresponds to a unique cell in the bayonet model.

Model Development

The model presented in above sections is formulated and dividing the height of the bayonets in 12 cells. Cell 1 corresponds to the base of the bayonet, where the flue gases enter. Cell 12 corresponds to the topmost cell of the bayonet. In the topmost portion of the bayonet, negligible heat loss in the top hemispherical section is assumed. The assumption is taken due to the complexity of the numerical representation. The thermal equilibrium in the 12th cell is constrained by equating the temperatures as indicated.

$$T_{C,12} = T_{1,12} = T_{2,12} = T_{A,12} \quad (9)$$

For each cell, the value of the residual is analysed to be minimize for each equation.

Simulation Specification

The attributes for coal selected, i.e., Thar Lignite are presented in Table 1. These numbers represent the PROXANAL and ULTANAL of an air-dried sample of Thar Lignite coal provided by Pakistan Council for Scientific and Industrial Research, PCSIR, Karachi, Pakistan. Thar coal was used as the indigenous feed for this study. The characteristics of Feedstocks used for the simulation are given in Table 2.

$$Q = 198.11C + 620.31H + 80.93S + 44.95A - 5153 \quad (10)$$

Proximate Analysis		Ultimate Analysis		Sulphur Analysis	
Element	Value (wt. %)	Element	Element	Value (wt. %)	Element
Moisture (wet basis)	8.5	C	54.57	Pyritic	1.46
		H	3.21		
Fixed carbon (dry basis)	25.83	N	1.07	Sulphate	1.47
		Cl	0		
Volatile Matter (dry basis)	53	S	4.39	Organic	1.46
		O	15.59		
Ash (dry basis)	21.17	Ash	21.17		

Table 1: Thar Coal Analysis.

COAL	Temperature	20	°C
	Pressure	34	barg
STEAM (Gasifying Medium)	Temperature	800	°C
	Pressure	34	barg

The Lower Heating Value of Thar Coal is evaluated by a correlation presented by Mason and Gandhi.

Table 2: Feedstock Condition for the Gasification.

Where,

Q=Gross Heating Value in Btu/lb,

C=wt % dry basis of carbon in ultimate analysis.

H=wt % dry basis of hydrogen in ultimate analysis.

S=wt % dry basis of sulphur in ultimate analysis.

A=wt % dry basis of ash in ultimate analysis.

Accordingly, the LHV of Thar coal is found to be 8956 Btu/lb or 4979 kcal/kg. The pyrolysis yield for Thar coal devised on the basis of ultimate analysis.

Results

A Study is carried out on the geometric aspect of the gasifier using the same Process Scheme. In this case, Feed conditions for both coal and steam are same. Length over diameter of the reactor has been decreased, due to which total gasifier volume is reduced. Number of bayonets in the reactor is also reduced by 41.6%. There will be some combustion in the lower section of the gasifier where steam is injected; therefore a lower temperature of steam at 800°C is used to keep the reaction temperature within limits.

Simulation results for the Thar Lignite Gasification using (L/D Ratio=5.75 and 4.6) in model are presented in Figures 4, 5 and 6. These results are based on the analysis of dry syngas after condensate removal from the raw syngas product stream.

From the results it is established that the tar contents and methane flow rate in product gas is dependent upon the geometry of the reactor i.e., increasing and decreasing effect of L/D Ratio. It is observed that as the L/D ratio increases from 4.6 to 5.75, the Condensate to Syngas ratio also increases but syngas yield decreases to a considerable extent due to lower conversion of carbon. Cold gas efficiency and Product split also got lower but the LHV of product gas is much higher when we have L/D ratio 5.75.

Figure 4 represents the results of different terminologies i.e., condensate/syngas ratio, conversion of C in gasifier and H₂/CO molar ratio. It is observed that the condensate/syngas ratio is decreasing as increase L/D ratio of the reactor. It can be deduced that there is inverse relationship between the L/D ratio of gasifier and the condensate/

syngas ratio. The Conversion of carbon in gasifier is showing optimum results by decreasing in the L/D ratio of gasifier. More precise results can be evaluated by inserting the values of L/D ratio in shorter intervals. H₂/CO molar ratio is showing increasing trend as with decrease in L/D ratio.

It is shown in Figure 5 that the Syngas yield is very low on increasing the L/D ratio. It is observed that the Syngas yield is showing tremendous increment at L/D ratio 4.6. Lowering the L/D ratio, therefore, increases the production of syngas via higher yield. This trend is continued in the case of cold gas efficiency and product split. These two quantities also increase by decrement in the L/D ratio. It means that lower L/D ratio is more feasible as it increases both the quality and the quantity of the syngas produced, hence lowering the % portion of the syngas burnt to provide process heat through the bayonets.

Conclusions

It was concluded that any alteration in L/D ratio resulted in lowering the values of syngas yield, cold gas efficiency and conversion of carbon in the gasifier. An Increasing trend of LHV Dry Syngas (kcal/kg) has been observed in case of increment of L/D ratio. Slight

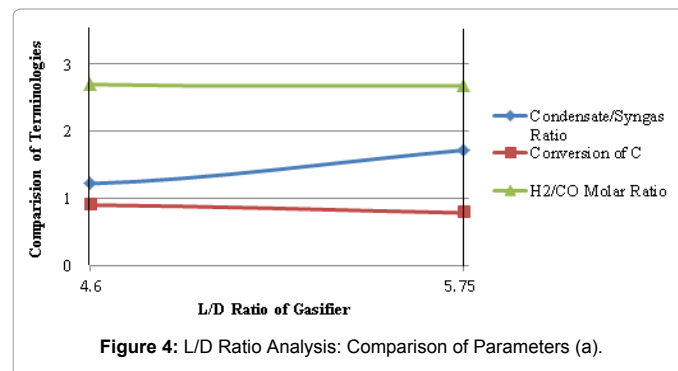


Figure 4: L/D Ratio Analysis: Comparison of Parameters (a).

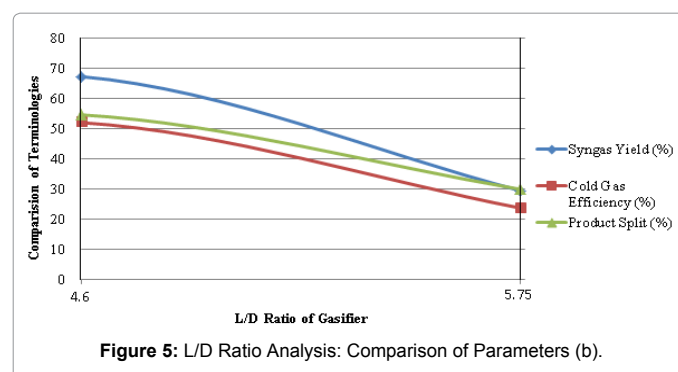


Figure 5: L/D Ratio Analysis: Comparison of Parameters (b).

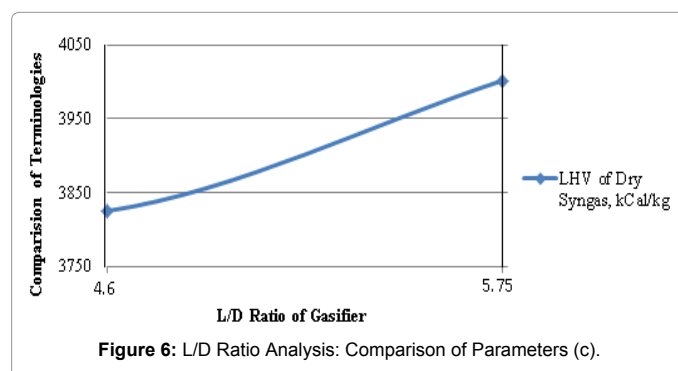


Figure 6: L/D Ratio Analysis: Comparison of Parameters (c).

decrease in H₂/CO ratio has been found. So, increment in L/D ratio is not advantageous for syngas production unless we are only concerned with the LHV of the syngas.

References

1. Bussman WR, Baukal CE, French KW (2005) Variable test furnace cooling. Paper presented at the ASME 2005 Summer Heat Transfer Conference collocated with the ASME 2005 Pacific Rim Technical Conference and Exhibition on Integration and Packaging of MEMS, NEMS, and Electronic Systems. pp: 291-304.
2. Chen PC, Yu CS, Chiu HM, Chyou YP, Chen HJ (2012) Process simulation study of coal gasification based multi-product plant with electricity and chemical products. *Asia Pacific Journal of Chemical Engineering* 7: S101-S111.
3. Hoffman Z (2005) Simulation and economic evaluation of coal gasification with sets reforming process for power production. Faculty of the Louisiana State University and Agricultural and Mechanical College in partial fulfillment of the requirements for the degree of Master of Science in Chemical Engineering In The Department of Chemical Engineering by Zachary Hoffman BS, Louisiana State University, USA.
4. Junaid Akhlaq FR, Alberto B (2015) Coal gasification by indirect heating in a single moving bed reactor. *Process development & simulation* 3: 635-665.
5. Lee H, Choi S, Paek M (2010) Interpretation of coal gasification modeling in commercial process analysis simulation codes. *Journal of Mechanical Science and Technology* 24: 1515-1521.
6. Mason DM, Gandhi KN (1983) Formulas for calculating the calorific value of coal and coal chars: development, tests, and uses. *Fuel Processing Technology* 7: 11-22.
7. Nayak R, Mewada R (2011) Simulation of coal gasification process using ASPEN PLUS. Paper presented at the Proceedings of the International Conference on Current Trends in Technology: Nuicone.
8. O' Doherty T, Jolly A, Bates C (2001) Analysis of a bayonet tube heat exchanger. *Applied thermal engineering*, 21: 1-18.
9. Rinard I, Benjamin B (1985) Great Plains ASPEN Model Development: Gasifier Model, Literature Review and Model Specification. Final Topical Report for the US Department of Energy, Morgantown, Energy Technology Center, Morgantown, WVt (2nd edn) Scientific Design Company, Division of the Halcon, SD Group, Inc., New York, NY, USA. pp: 19163-11782.
10. Sudiro M, Pellizzaro M, Bezzo F, Bertucco A (2010) Simulated moving bed technology applied to coal gasification. *Chemical Engineering Research and Design* 88: 465-475.
11. Sudiro M, Zanella C, Bertucco A, Bressan L, Fontana M (2010) Dual-Bed Gasification of Petcoke: Model Development and Validation. *Energy & Fuels* 24: 1213-1221.
12. Wen C, Chaung T (1979) Entrainment coal gasification modeling. *Industrial & Engineering Chemistry Process Design and Development* 18: 684-695.
13. Wen C, Chen, H, Onozaki M (1982) User's manual for computer simulation and design of the moving-bed coal gasifier. Final report: Department of Chemical Engineering, West Virginia University, Morgantown, USA.