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Studies of Hydrodynamic Behaviour and Syn-Gas Production from Biomass Solid Wastes Using Fluidized Bed Gasifier: An ASPEN Plus Simulation

Tripathy Rajesh¹ and ^{*}Sahoo Abanti²

Department of Chemical Engineering, National Institute of Technology, Rourkela-769008, Odisha, INDIA

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Abstract : Fluidized bed gasification is one of the potential techniques for production of clean and ecofriendly fuel. ASPEN PLUS simulator is a strong tool for investigating the behavior of a process and it can be readily used to access various aspects like feasibility of an operation, effects of operating parameters on the performance of a gasifier. In the present work, the simulator has been used to simulate the effect of different system parameters (viz. Steam Flow rate, steam to biomass ratio, air flow rate, temperature, equivalence ratio, pressure) on the reaction kinetics mainly, on the product gas composition and carbon conversion efficiency of the fluidized bed gasification. Again hydrodynamic behaviour of the Fluidized Bed Gasifier (cold model) has been carried out with respect to different static bed heights and particle sizes of the bed material. The dolomite has been used as a bed material. Temperature was observed to be the most sensitive kinetic parameter thereby implying as the important aspect of gasification when operated under atmospheric pressure. Use of steam as a gasifying agent was observed to improve the syn-gas production.

Keywords: Fluidized bed gasification, Carbon conversion efficiency, equivalence ratio, steam to biomass ratio and ASPEN PLUS, Syn-gas.

Introduction

Gasification refers to a group of processes which highlights the conversion of solid or liquid fuels into a combustible gas in the presence or absence of a gasifying agent. The concern for climatic variations has triggered the interest in biomass gasification using fluidized bed gasifiers as one the popular options. Biomass being readily available, economic and carbon dioxide neutral is one the upcoming prospects for eco-friendly techniques and it is one of the most effective re generative source of energy. Gasification definitely has certain important advantages over direct combustion.

When the fuel is processed, the volume of gas obtained from gasification is significantly less as compared to that of combustion. The reduced volume of gas needs smaller equipment which results in reduced costs. Gasification definitely is an attractive option for remote locations. However one of the important shortcomings of gasification involves the reduced carbon conversion efficiency due to which a certain part of the fuel energy remains in the char ^[3]. The objective of this study is to develop simulation using ASPEN PLUS which will be

capable of estimating the steady-state performance of a fluidized bed gasifier by considering the reaction kinetics which helps to find out an optimum and more effective process operating condition to produce the maximum output. It makes more easy and efficient design of a gasifier on the basis of the simulation results.

Material and Methods

It is normally carried out by the reaction of fuel such as coal, biomass, oil or coke with a minimum amount of oxygen often in combination with steam. The heat liberated from the exothermic reactions of fuel and oxygen maintains the gasifier at the operating temperature and drives the endothermic gasification reactions taking place inside the gasifier ^[11]. Steam can be used as the gasifying agent only if an external source of heat is provided which drags the endothermic reactions forward.

Donald L. Klass^[5] has shown that Biomass gasification processes could be divided into three categories viz. Pyrolysis, Partial oxidation and Reforming ^[2]. If temperature is sufficiently high the process is known as the pyrolysis and the primary products from pyrolysis of biomass are gases. The next step is partial oxidation which utilize less than stoichiometric amount of oxygen required. The last section is the reforming section where conversion of hydrocarbon gases and vaporized organic compounds to hydrogen containing compounds takes place.

Gasification processes can be designed in such a way that the exothermic and endothermic reactions are thermally balanced. It is not possible to control the process as there is such a competition among so many reactions. Thus there is a need for the proper combination of temperature, pressure, reactant and recycle product, feed rates, reaction time and oxygen to steam ratio.

Drying, pyrolysis and reduction absorb heat provided by the exothermic combustion process. In drying, the moisture from the solid fuel evaporates. The pyrolysis or de-volatilization process separates the water vapor, organic liquids and non-condensable gases from the char or solid carbon of the fuel. The combustion reactions oxidize the fuel constituents while the gasification process reduces them to combustible gases in an endothermic reaction^[3].

The pyrolysis process starts around 350° C and then shoots above 700° C. The composition of the evolved products depends upon temperature, pressure and gas composition during de-volatilization. In pyrolysis, the volatile components break down first and then evaporate.

It can be shown by a general reaction as follows. Biomass + heat \rightarrow char + gases + vapors or liquid

The vaporized product contains tar and other polyaromatic hydrocarbons. The tar produced poses a major hindrance in the smooth running of the gasifier. Pyrolysis generally produces gases like (H_2 , CO, CH₄, H_2 O, CO₂.), Tar (a black, viscous and corrosive liquid) and Char, a solid residue containing carbon. In combustion, oxidation of char takes place which practically deals with all the thermal energy needed for endothermic reactions. The following reactions take place in combustion.

$$C + O_2 \rightarrow CO_2 \tag{1}$$
$$H_2 + 0.5 O_2 \rightarrow H_2O \tag{2}$$

Gasification mainly involves the following series of reactions.

Water gas reaction	
$C + H_2O \rightarrow H_2 + CO$	(3)
Boudouard reaction	
$CO_2 + C \rightarrow 2CO$	(4)
Shift conversion	
$\rm CO + H_2O \rightarrow CO_2 + H_2$	(5)
Methanation	
$C + 2H_2 \rightarrow CH_4$	(6)

It is found that different types of beds are being used by different investigators to check the quality as well as the amount of syngas production. The researchers have varied the operating parameters as shown in the comparison table (Table 1). Fluidized bed gasifier is observed to be the most effective method for production of synthesis gas by gasification process ^[3]. Different parameters studied for fluidized bed gasification are also shown in Table 1. The overall performance of the fluidized bed gasifier is found to be satisfactory in comparison with other types.

Effect of Feed Properties on Gasification: The composition of gas obtained from the gasifier depends upon the feed composition, gasifying medium, operating pressure, temperature, moisture content of the feed and mode of contact of reactants inside the gasifier.

Parameters	Fixed/moving	Fluidized bed	Entrained bed
	bed		
Feed size	<51mm	<6mm	<0.15mm
Tolerance of fines	Limited	Good	Excellent
Tolerance for coarse	Very good	Good	Poor
Exit gas temperatures	450-650 ⁰ C	800-1000 ⁰ C	>1990 °C
Feed stock tolerance	Low rank coal	Low rank coal and	Any coal including
		excellent for biomass	caking but unsuitable
			for biomass
Oxidant requirements	Low	Moderate	High
Reaction zone temperature	1090 ⁰ C	800-1000 ⁰ C	>1990 °C
Steam requirement	High	Moderate	Low
Nature of ash produced	Dry	Dry	Slagging
Cold gas efficiency	80%	89.2%	80%
Application	Small capacities	Medium size capacities	Large capacities
Problem area	Tar production	Carbon conversion	Raw gas cooling
	and utilization of		
	fines		

 Table 1

 Some relative operational characteristics regarding gasification ^[3]

The reactivity in gasification increases with pore volume and surface area of the feed. The particle size and porosity of feed have significant effects on the kinetics of gasification. The reactivity of fuel and its conversion to char depends upon its volatile matter content. Fuels or feed with high volatile matter are more reactive, produce less char and conversion to gas is better. Biomass feedstock generally contain high amount of volatile matter (about 25%).The moisture content is a decisive factor for the gasification process since high moisture content of the feed can lower the temperature inside the gasifier thereby hindering the kinetics of gasification reactions which needs high temperature because of endothermic nature. Therefore the feedstock should have an optimal moisture content of 5-10%.

Design Considerations

Gasifier Efficiency: The performance of a gasifier is often expressed in terms of its efficiency, which can be defined in two ways: cold gas efficiency and hot gas efficiency. The cold gas efficiency is used if the gas is used for running an internal combustion engine in which case the gas is cooled down to the ambient temperature and tar vapors are removed. It is defined as

$$\eta = \underbrace{\bigwedge_{b}^{s} * q_{s}}_{M_{b}} \underbrace{K_{b}}_{b} \underbrace{K_{b}} \underbrace{K_{b}}_{b} \underbrace{K_{b}}_{b} \underbrace{K_{b}}_{b} \underbrace{K_{b}}_{b}$$

For thermal applications, the gas is not cooled before combustion and the sensible heat of the gas is also used. The hot gas efficiency is defined as

$$\eta_{geff} = \frac{\sum_{g \neq g} * q_{g} + H_{sensible}}{\sum_{g \neq g} * c_{g}}$$
(8)

Where, Vg = gas generation rate (m^3/sec); M_b = fuel consumption rate (kg/sec),

qg= heating value of the gas (kJ/m^3) ; C_b= heating value of fuel (kJ/m^3)

Equivalence Ratio: It is defined as the ratio of actual airfuel ratio to the stoichiometric air-fuel ratio. An excessive low value of ER (ER<0.2) results in several problems including incomplete gasification, excessive char formation and low heating value of product gas. On the other hand if ER>0.4 then the problems of excessive formation of products of complete combustion rather than the desired ones of CO and H₂ are encountered. Therefore an optimum equivalent ratio of 0.2-0.3 has to be maintained ^[3].

Bed Materials: The bed material in case of fluidized bed gasifier consists mainly of inert solid particles and some fuel particles at different stages of gasification. In case of biomass gasification silica sand or magnesium oxide is used as inert bed material. The bed materials besides serving as a heat carrier can also catalyze the gasification

reaction by increasing the gas yield and reducing the tar formation.

Experimentation

The schematic diagram of the gasifier (Cold Model) has been shown in Fig.-1. The hydrodynamic behavior study was carried out in the laboratory by experiments where set up consists of a Cold Model Gasifier made up of Acrylic material as shown in Fig.-2. Different bed materials which are to be used in the real mode i.e. hot model unit of gasifier were studied in the cold model unit. The hydrodynamic characteristics mainly pressure drop and minimum fluidization of these bed materials were studied in the cold model unit by varying different system parameters. The same operating conditions are to be maintained in the hot model unit, where the actual gasification reactions will be carried out. Thus these operating conditions will be the controlling factor for determining the compositions of the product gas from the Hot Model unit. In the present work Dolomite has been used as the bed material whose properties are listed in Table 2.Particle diameter was calculated by sieve analysis, density determined by taking a measured quantity of the selected size of particle in a known volume and the specify as well as the voidage was also calculated by simple logical methods with the help of volume of water taken in the free space available. Three different sizes of bed materials (viz. 1.193 mm, 2.18 mm and 2.58 mm) were taken for analysis. The pressure was maintained constant at 1atmosphere.



Figure 1: The schematic diagram of the Cold Model



Figure 2: Gasifier cold model in laboratory

Properties	Values
Particle diameters (d_p)	1.193mm,2.18mm,2.58mm
Density of particle (ρ_p)	2860 kg/m^3
Voidage ($\boldsymbol{\varepsilon}$)	0.4
Sphericity (φ)	0.75

Table 2Properties of bed material for the gasifier



Figure 3: Pressure Drop versus Bed height at minimum and turbulent fluidization conditions for sample 1 dolomite



Figure 5: Pressure Drop versus Bed height at minimum and turbulent fluidization conditions for sample 3 dolomite



Figure 7: Pressure Drop across the bed versus Bed height

On studying the variation of pressure drops across the bed at minimum and turbulent fluidizations, it was

Variation of pressure drop against the bed height for both minimum fluidization and turbulent fluidization is shown in Fig.-3 and 4. Again pressure drop variation against bed height has been shown in Fig.-5 and 7 for different fluidization conditions and for different particle sizes respectively. Fluidization velocity has also been varied with the bed height (Fig.-6).



Figure 4: Pressure Drop versus Bed height at minimum and turbulent fluidization conditions for sample 2 dolomite



Figure 6: Fluidization velocity versus Bed height

observed that higher pressure drops are obtained across the bed when there is a shift from minimum to turbulent fluidization (Figure 3, 4 and 5). Dolomite with particle diameter 1.193mm has higher fluidization velocities as compared to the sample with 2.18mm particle diameter because as the particle size increases the void fraction of the bed increases this in turn reduces the resistance and the bed fluidizes even by applying less velocity. But when the particle diameter increases further from 2.18mm to 2.58mm, the particle weight is not counterbalanced by the buoyant force and the bed materials requires higher fluidization velocity (Figure 6). Hence the fluidization velocities decreases from particles of dp=1.193mm to particles of dp =2.18mm. But again fluidization velocity increases with particles of dp=2.58mm. In all the above cases it is observed that the pressure drop across the bed follows a steady pattern when the bed height is 4 cm which is approximately 50% of the bubble cap height (Figure 7). 50% of the height of bed material height is found suitable because at that height weight of bed materials are perfectly counter balance with the fludizing media supplied and the flow rate is enough to use in real gasification operation, maximum air supply to the process leads the process to combustion and dilution of the product gas^[3]. It was observed that all the three samples can be fluidized but are not suitable for gasification because they need high fluidization velocities and high mass flow rates of air which might affect the quality of product gas in gasification reactions. That is why the fludisation velocity of a biomass should be such that the air should be sufficient to bubble the bed material for enhancing the gasification reaction and stoichiometrically as well. The higher pressure drop is observed across the bed when there is a shift from minimum to turbulent fluidization because the bed is allow to expand more and the size of air bubble formation is quit bigger than the previous condition which leads to fluctuation in pressure drop.

In the present case, the experimentation basically is restricted to the study of bed hydrodynamic characteristics in the Cold Model unit of fluidized bed gasifier. Hot model experimentation is taken as the future work for the present article.

Simulation and Modeling: ASPEN PLUS simulator provides an opportunity to check the feasibility of a process, to study and investigate the effect of various operating parameters on various reactions. It is a strong tool for simulation studies and helps in analyzing the outcome of a process.

ASPEN PLUS simulation: According to Pengmei LU et al.^[2] biomass gasification models can be divided in two ways

Kinetic model: The reaction conditions are simulated at different times and sites which makes it suitable for reactor amplification design and optimization of operation parameters.

Equilibrium model: Only end reaction product distribution is predicted. In this particular simulation both the reaction kinetics parameters and bed hydrodynamics aspects are considered. The following assumptions are made in modeling the gasification process.

Process is assumed to be isothermal and steady state. Biomass de-volatilization is instantaneous in comparison to char gasification. Particles are spherical and are not affected in course of the reaction based on the shrinking core model ^[4]. Char comprises only of carbon and ash. Char gasification initiates in the bed and ends up in the freeboard. Char with the waste tar looks like mud. As certain parameters for solid modeling are not available in ASPEN PLUS, liquid modeling is considered for this mud like char and waste tar produced from the biomass gasification rather than solid modeling.

The simulation is carried out with power-law kinetics. The residence time for reactants is sufficiently high to reach chemical equilibrium.

Kinetic Parameters used in ASPEN PLUS Simulation

Gasification reactions and their kinetic parameters are given in Table-3 as follows. Characteristics of saw dust are given in Table 4. The characteristic of biomass was foun out in laboratory by Total Organic Carbon Analyzer and CHNS Analyzer Elementar Analysen Systeme, Germany, Vario EL.

ASPEN PLUS Modeling

The different stages considered in ASPEN PLUS simulation are decomposition of the feed, volatile reactions, char gasification, and gas–solid separation.

Biomass Decomposition: The ASPEN PLUS yield reactor, RYIELD, was used to simulate the decomposition of the feed. In this step, biomass is converted into its components including carbon, hydrogen, oxygen, sulfur, nitrogen, and ash, by specifying the yield distribution according to its ultimate analysis^[3,5].

Reactions	Rate constant (sec ⁻¹ atm ⁻¹)	Activation energy (kJ/mole of carbon)
$C + H_2O \rightarrow H_2 + CO$	6474.7	13130
$CO_2 + C \rightarrow 2CO$	6474.7	17250
$CO + H_2O \rightarrow CO_2 + H_2$	6474.7	4198
$C + 2H_2 \rightarrow CH_4$	6474.7	7481
$C + 0.5 O_2 \rightarrow CO$	0.046	110.50
$C + O_2 \rightarrow CO_2$	0.046	393.77

 Table 3

 Gasification reactions and their kinetic parameters ^[3]

Table 4Characteristics of saw dust

Moisture content (%)	7.8	
Proximate analysis (dry weight %)		
Volatile matter	82.24	
Fixed carbon	17.17	
Ash	0.50	
Ultimate analysis (dry weight %)		
Carbon	52.55	
Hydrogen	7.08	
Oxygen	41.00	
Nitrogen	0.16	
Sulfur	0.57	

Volatile Reactions: The ASPEN PLUS Gibbs reactor, RGIBBS, was used for volatile matter combustion under the assumption that volatile reactions follow the Gibbs equilibrium. Carbon will partly constitute the gas phase, which takes part in de-volatilization, and the remaining carbon comprises part of the solid phase (char) and subsequently results in char gasification^[6]. A SEPARATION COLUMN model was used before the RGIBBS reactor to separate the volatiles and solids in order to perform the reactions.

Char Gasification: CSTR reactor and RCSTR were used to perform char gasification by using reaction kinetics. Then the reactor is divided into two regions, main bed and freeboard. Each region was simulated by one RCSTR. In these small reactors the following hydrodynamic and kinetic parameters, such as superficial velocity, voidage, fractional pressure of oxygen and steam were assumed constant. The number of the elemental reactors depends on the residence time, the reactor dimensions and the operating conditions whereas the mentioned parameters can be considered constant ^[4,7, 8]. Operating parameters for the experiment are shown in Table 5. The parameter chosen for the simulation in the Table 5 is consider as a reference from the literature that the range of gasification operation, one can vary the parameters and simulate for the particular operation condition ^[3] Simulation flow sheet for the fluidized bed gasification is shown in Figure 8.

Results of Simulation Approach and Experimentation Model : The empirical formula of the biomass sample was found to be $CH_{1.68}O_{0.62}$. Thus the reaction can be written as follows.

$$CH_{1.68}O_{0.62} + 1.11 O_2 \rightarrow CO_2 + 0.84 H_2O$$

The effects of pressure, temperature, steam to biomass ratio and equivalence ratio on product gas composition and carbon conversion efficiency were carefully studied. Simulation trials were conducted by varying the steam flow rates thereby changing the steam to biomass ratio whereas the biomass flow rate and all other parameters were kept constant.



Figure 8: Simulation flow sheet for fluidized bed gasification

Fluidized Bed Reactor		
Temperature (⁰ C)	700-1000	
Pressure (bar)	1.05	
Bed diameter (mm)	40	
Freeboard diameter	60	
Height (mm)	1400	
Air		
Temperature (⁰ C)	65	
Flow rate (m ³ /hr)	0.5-0.7	
Steam		
Temperature (⁰ C)	145	
Flow rate (kg/hr)	0-1.8	

Table 5Operating parameters for the simulation



Figure 9: Product gas composition versus steam to biomass ratio



Figure 11: Product gas composition versus air flow rate











Figure 12: Product gas composition versus temperature



Figure 14: Product gas composition versus equivalence ratio



Figure 15: Product gas composition versus pressure variation

Figure 16: Carbon conversion efficiency with steam to biomass ratio

The product gas composition was found out by varying the different system parameters with the help of ASPEN PLUS Simulation which are shown through Figure 9 to Figure 15. Again carbon conversion efficiency was observed to change with the steam to biomass ratio by simulation which has been shown in Figure 16.

A decreasing trend in the product gas composition against the steam to biomass ratio (in lower range) was observed for all the constituents (Figure 9) but the decreasing effect was much significant when comparatively higher values of steam were used (Figure 10). The extremely low composition of CO_2 can be attributed to the simplifications used in the simulation. The decreasing trend is expected for CO_2 but the reduction in composition for CO may be due to the water gas shift reaction where the CO formed reacts with steam and convert to CO_2 .

The effect of air flow rate was studied on product gas composition (Figure 11). As expected the compositions of H₂ and CO started reducing but the reduction wasn't prominent so the effect of air flow in the form of equivalence ratio was analyzed and significant reduction was observed (Figure 14). The effect of equivalence ratio on carbon conversion efficiency (Figure 13) showed the closest resemblance to the theoretical predictions. Initially when the equivalence ratio is increased the carbon conversion increases but after reaching a maximum, there is a reduction which may be attributed to the formation of complete combustion products like CO₂ and H₂O rather than CO and H₂. The optimum value of equivalence ratio was found to be 0.23 for maximum carbon conversion. Temperature has the most profound impact on product gas composition since gasification is a temperature controlled reaction.

The gasification reactions being endothermic in nature need high temperature to drive them forward to completion. It was observed that after 900^oC saturation is obtained in the composition of product gas components (Figure 12). The products of endothermic reactions H_2 and CO showed an increasing trend when the temperature was raised but CO₂ and CH₄ showed descending trends as these are obtained from exothermic reactions. On increasing the pressure, CO and H₂ compositions kept on decreasing which indicates that hydrogen is achieved as the main product only when the pressure decreases. Atmospheric pressure has been used for hydrogen extraction (Figure 15). The variation of carbon conversion efficiency with steam to biomass ratio has shown an increasing trend initially. Then a descending trend and again an increasing trend after some time has been achieved (Figure 16). The response can be comprehended as the production of CO increases initially with increase in steam flow rate due to water gas reaction but then shift reaction takes place which consumes CO thereby converting it into CO₂ which would react with char to produce CO again.

Conclusion

A simulation study using ASPEN PLUS was performed considering only the kinetic parameters for sawdust sample where it's proximate and ultimate analysis were used. The effect of various operating parameters was studied on the product gas composition and carbon efficiency. Various assumptions conversion were incorporated to make the simulation feasible. Some of the results obtained strayed away from the standard pattern due to the absence of a more realistic and rigorous model. However some of the results obtained were quite close to the theoretical predictions. The actual process is a lot more complicated due to tar formation and ash agglomeration which does have an impact on the performance of the gasifier. The steam to biomass ratio was found to be in the range of (0.1-1) for obtaining tangible values of product gas composition. Steam being used in the temperature range of (120-150) ⁰C should be used at comparatively higher flow rates for steady operation of a gasifier.

The temperature should be in a range of $(700-900)^{0}$ C for making a comparative analysis of composition of various product gas components. The equivalence ratio should be in a range of (0.18-0.24) to obtain high carbon conversion efficiency of (85-89) %. If the ratio is lower than 0.18 that would lead to incomplete gasification and if it is higher than 0.24 then it would lead to formation of complete combustion products like CO₂ and H₂O. Pressure should be close to atmospheric pressure for production of CO and H₂.

There is a competition between the several gasification reactions to reach completion so it is very difficult to access the product gas composition as it also depends upon the operating parameters. The purpose of gasification dictates the presence or absence of a gasifying agent. ASPEN PLUS simulator provides a great deal of help in accessing the performance of a unit operation. It gives various insights about optimizing the various process parameters. It also assists in making cost estimations, judging the economy of an operation and making sensitivity analysis while finding out the critical components which mainly affect a process. Through the bed hydrodynamics study with dolomite as the bed material and with different particle sizes it was observed that for the real model application of gasification the particle size of dolomite should be less than 1.193 mm to achieve proper fluidization conditions and maintain the better quality of gasification products.

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