AIR AND OXYGEN GASIFICATION SIMULATION ANALYSIS OF SAWDUST

by

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Gasification is the conversion process of low-grade solid fuel into gaseous fuel by thermo-chemical reactions. In this paper air gasification and oxygen gasification simulation of sawdust is carried out using FACTSAGE 6.3 software. The effect of temperature and equivalence ratio (ϕ) on producer gas composition is analysed. Combustible gas compositions (H_2, CO and CH_4) are found out at different operating conditions for air and oxygen gasification separately. Temperature range is 200 - 1200 °C and ϕ value varied from 0.3 - 0.6. Gas heating values (HHV & LHV) carbon conversion efficiency (CCE) and cold gas efficiency (CGE) are calculated. In air gasification, maximum HHV of 5.96 MJ/Nm^3 is reached at 700 °C for ϕ=0.3 and in oxygen gasification, 9.85 MJ/Nm^3 is attained at 800 °C and ϕ=0.3. The maximum cold gas efficiency of 84.37 and 84.73% reached by air and oxygen gasification respectively at 1200°C for ϕ=0.3.

Keywords: *Sawdust, Air gasification, Oxygen gasification, Simulation, FACTSAGE.*

1. Introduction

Gasification is an old technique practised in the early 19th century to illuminate street with coal gas. The energy crisis in 1970 gave re-birth to gasification technology and demand for clean energy stimulates the research and development. Gasification is the conversion process of carbonaceous material into combustible gas by partial oxidation at high temperature [1]. Heat and combustible gases are the main products of gasification, ash, char, tar and non-condensable gases are by-products. Char is the carbonaceous solid residue of biomass, tar is a mixture of phenol, polycyclic aromatic hydrocarbons and heterocyclic hydrocarbons [2]. The main gaseous products formed during gasification are carbon monoxide, carbon dioxide, hydrogen, methane, water vapour and nitrogen from the air [3,4]. During gasification process, fuel undergoes four stages namely drying, pyrolysis, gasification and combustion [5,6]. Biomass and coal are the main fuel for the gasification process.

Biomass includes wood, agricultural residues, municipal solid waste and wastes from food processing and many more. Biomass is an attractive fuel in the developed country, it is renewable, low in sulphur content and CO_2 neutral [7]. It is utilised for chemical raw materials production, power generation and production of alternate fuel [8]. Direct combustion is the traditional way of utilising biomass; it causes more pollution and has low energy conversion efficiency [3, 4]. Electricity can be generated with single fuel or mixture of fuels by gasification-based power generation technique, has higher efficiency than conventional pulverised fuel combustion method [9]. Biomass contains volatiles, fixed carbon, ash and moisture, on heating moisture removed around 120°C. Devolatisation takes place up to 350°C and char gasification occurs above 350°C [10]. All type of biomass has more oxygen and hydrogen content and less carbon than coal, it is indicated by higher volatile and moisture content [7]. Due to high reactivity, biomass releases more volatile matter which improves oxidation and gasification reactions [11]. Gasification is an endothermic process, heat is supplied by partial oxidation of fuel in case of auto-thermal and external heat is supplied for allo-thermal gasification [10]. Operating temperature of gasifier varies from 200 - 1200°C and pressure ranges from atmospheric pressure to 2.4 MPa. Biomass air gasification produces gases with LHV of 4 - 6 MJ/Nm^3 with 8 - 14% of H_2 but highly diluted with N_2 [12,13]. Oxygen gasification provides the medium gas heating value of 10 - 12 MJ/Nm^3 and free from tar, the steam gasification heating value is in the range of 10 - 16 MJ/Nm^3 with 30 - 60% of H_2 content and superior carbon conversion [14 - 16].

Shayan et al [17] studied gasification of wood and paper by stoichiometric equilibrium model with the gasifying mediums - air, O_2 enriched air, O_2 and steam. The calorific value of gas, energy efficiency, exergy efficiency and exergy destruction are found. For wood, the gas calorific value of 5.3 and 11.2 MJ/Nm^3 are obtained in air and steam gasification respectively. Shweta and Pratik [18] studied the effect of moisture content, steam to biomass ratio and equivalence ratio on gas composition in a downdraft gasifier for combined air-steam gasification. Equilibrium modelling results are validated with experimental values. Gas composition, calorific values and cold gas efficiencies are calculated. Karl et al [19] studied gasification of switchgrass in oxygen and steam blown fluidised bed gasifier, for equivalence ratio 0.21 - 0.38 and temperature up to 900°C. An equilibrium model is developed by Aspen plus software, gas composition (H_2, CO, CO_2, CH_4, C_2H_6, C_2H_4, C_2H_2, HCN and NH_3), heavy tar content, char content, gas yield, HHV, CCE and CGE are calculated. Niu et al [20] gasified municipal solid waste (paper, wood, textile and kitchen garbage) with O_2 in fixed bed gasifier. Gas composition, char, tar and gas lower heating value are found for 700-900°C and ϕ=0.14 - 0.32. LHV of gas is in the range of 6 - 10 MJ/Nm^3. In the present study, maximum LHV of 9.24 MJ/Nm^3 is obtained in oxygen gasification at 1200°C for ϕ=0.3.

In the present work, gasification of sawdust is carried out by FACTSAGE 6.3 software for air and oxygen mediums. Non-stoichiometric equilibrium model based on Gibbs free energy minimisation with Lagrange multiplier iterative method is used to find out the equilibrium composition of end products for temperature range 200 - 1200°C and ϕ value 0.3 - 0.6. The objective function of the model is given by Eq. (1), it is subjected to mass balance and non-negativity of the number of moles to find end composition.

$$G / RT = \sum_{j=1}^{n} n_j \left[\frac{G^0}{RT} + \ln \frac{n_j}{\sum n_j} \right] \tag{1}$$

Where, G – Total Gibbs energy kJ

G^0 – Gibbs energy of pure component kJ

R – Universal gas constant kJ/ kmol K

n_j – Number of moles of component j

To validate the model, simulation results of rice husk air gasification and steam gasification are compared with experimental work of Karmakar et al [21] and Loha et al [22] respectively. RMS values are calculated using Eq. (2), Karmakar et al [21] used 50 kg/hr bubbling fluidised bed gasifier and sand as bed material with the mean diameter of 0.334 mm. The reactor is made up of carbon steel, cylindrical in shape with an inner diameter of 0.5m and 1m in height. Loha et al [22] used laboratory scale fluidised bed gasifier of 50 mm diameter and 1200 mm in height. Sand used as bed material and steam as a gasifying agent, heat is supplied by an electric furnace.

$$\text{RMS} = \sqrt{\frac{\sum_J^N (\text{Experiment} - \text{Simulation})^2}{N}} \qquad (2)$$

Where N is the number of gas components.

2. Methodology

Elemental composition of fuel, the quantity of air, temperature and pressure of gasification are the input details for simulation. Basic elements of sawdust are C, H, O, N, and S; nitrogen and sulphur are generally neglected in gasification process because of its low content in fuels [10]. In order to analyse the effect of temperature on gas composition, temperature varied from 200 to 1200°C by 100°C, equivalence ratio value varied from 0.3 to 0.6 by 0.05 for both air and oxygen gasification. The lower limit of ϕ value is decided by the minimum quantity of gasifying medium required to burn the fuel and to produce sufficient heat for endothermic reactions [23]. When ϕ value < 0.3, it is difficult to run the gasifier due to insufficient gasifying medium and if $\phi > 0.6$, it leads to combustion instead of gasification. Calculated sawdust stoichiometric oxygen to fuel ratio and air to fuel ratio are 1.22 and 5.29 respectively. Combustible gas composition (H_2, CO and CH_4), gas heating values (HHV and LHV), CCE, CGE are found. Proximate and ultimate analysis details of sawdust and rice husk are shown in Table 1.

Table 1. Proximate and ultimate analysis of sawdust and rice husk

S.No	Fuel	Proximate Analysis				Ultimate Analysis				
		Volatile matter	**Fixed carbon**	**Moisture**	**Ash**	**C**	**H**	**N**	**O**	**S**
1	Sawdust [24]	76.1	8.9	14.6	0.40	44.96	5.83	3.10	45.5	0.61
2	Rice husk [21]	55.54	14.99	9.95	19.52	38.43	2.97	0.49	36.36	0.07
		combustible								
3	Rice husk [22]	70.53		11.5	8.5	49.07	3.79	0.63	46.42	0.09

2.1. Method of data processing

Higher heating value (HHV) of the gas mixture is calculated from final gas composition given by Xiao et al [25].

$$\text{HHV} = ((H_2\% \times 30.52 + CO\% \times 30.18 + CH_4\% \times 95) \times 4.1868)\ \text{kJ/Nm}^3 \qquad (3)$$

Lower heating value (LHV) of the gas mixture is calculated from final gas composition given by Cheng et al [26].

$$\text{LHV} = (CO\% \times 126.36 + H_2\% \times 107.98 + CH_4\% \times 358.18)\ \text{kJ/Nm}^3 \qquad (4)$$

Where gas components are mentioned in mole percentage.
Gas yield is defined as the flow rate of total inert-free gas produced to flow rate of the dry and ash free value of feedstock [27]. Gas yield (Y) is calculated from Eq. (5) given by Ngo et al [28].

$$Y = \text{Volume of gas / Mass of sawdust } Nm^3/kg \quad (5)$$

Lower heating value of sawdust is calculated from Eq. (6) given by Proll and Hofbauer [29].

$$LHV_{sawdust} = (34835\ C + 93870\ H - 10800\ O + 6280\ N + 10465\ S)\ kJ/kg \quad (6)$$

Where saw dust elemental components are mentioned in mass fraction.

Cold gas efficiency is the ratio of energy present in the syngas to the energy present in the sawdust. Hydrogen production is indicated by cold gas efficiency [30]. Carbon conversion is defined as the total carbon content of the gas produced (CO, CO_2 and CH_4) to the total carbon content of feedstock [27]. Cold gas efficiency and carbon conversion efficiency are calculated from Eq. (7) and (8) given by Cheng et al [26].

$$CGE = (LHV_{gas} / LHV_{sawdust}) \times Y \times 100\ \% \quad (7)$$

$$CCE = [12 \times Y \times (CO\ \% + CH_4\ \% + CO_2\ \%) / (22.4 \times C\ \%)] \times 100\% \quad (8)$$

Where gas components are mentioned in mole percentage and carbon in mass percentage.

3. Result and discussion

Biomass gasification influenced by temperature, pressure, fuel composition, moisture content, type of gasifier, gasifying medium and residence time [31,32]. The analysis of gas composition is done with respect to temperature and equivalence ratio. Oxygen gasification and steam gasification are the common methods followed to improve gas heating value; product gas is free of nitrogen when oxygen and steam are gasifying mediums. For steam, the process becomes allo-thermal, heat has to be supplied externally [33]. Oxygen gasification produces a high yield of hydrogen but the separation of oxygen from air is an energy-intensive process [30].

3.1. Effect of temperature on gas composition

The operating temperature of the gasifier is limited by the volatile content of the fuel, production of NO_x, ash fusion temperature and material used [34, 35]. Gasification temperature is less than 900°C for biomass due to the presence of high volatile matter [36]. Temperature affects the gas composition, carbon conversion, amount of char formation, gas yield, gas heating value and gas efficiencies. Performance of gasifier depends on the thermodynamic behaviour of reactions and balance between endothermic and exothermic reactions [27]. Temperature influences Boudouard reaction, steam reformation and water-gas shift reaction [10]. Gaseous product composition of air and oxygen gasification are comparable but wide variation in mole percentage occurs due to the absence of nitrogen in oxygen gasification. CO formation takes place during the devolatisation stage by carbon partial oxidation, Boudouard reaction and primary water gas reaction [37, 38]. Chemical reactions taking place in the gasifier are listed in Table 2. Combustible gas composition variation with the operating condition in air and oxygen gasification is shown in Fig. 1.

In air gasification, H_2 increases up to 700°C for ϕ=0.3 - 0.45 and for other ϕ values it increases up to 600°C. In oxygen gasification, H_2 increases up to 800°C for ϕ=0.3 and for other ϕ values it increases up to 700°C. The decrease of H_2 after peak value is explained by Le Chatelier's principle, above 900°C hydrogen production decreases due to the exothermic behaviour of water-gas shift reaction [10]. Maximum H_2% of 20.81 and 33.84% are attained at ϕ=0.3, in air and oxygen gasification respectively.

CH_4 content decreases except for initial temperature rise (200 - 300°C), the maximum value of 3.99% reached at ϕ=0.3 in air gasification. CH_4 content increases up to 400°C, the maximum value of 8.49% reached at ϕ=0.3 in oxygen gasification. The variation of the CH_4 composition is due to production and consumption of methane in exothermic reactions at low temperature [39]. Rise in temperature decreases CH_4 due to further cracking and reforming reactions [40]. The extended increase of CH_4 in oxygen gasification is explained by the effect of temperature on methane production depends on gasifying agent [11]. Increase in temperature increases CO content for all equivalence ratio, the maximum value of 28.73 and 47.40% are attained at 1200°C for ϕ=0.3 in air and oxygen gasification respectively. CO% is less than 4% up to 600°C, low CO concentration is due to water gas shift reaction. CO content increases with the rise in temperature due to Boudouard reaction and primary water gas reaction [41 - 43].

Table 2. Gasification reactions

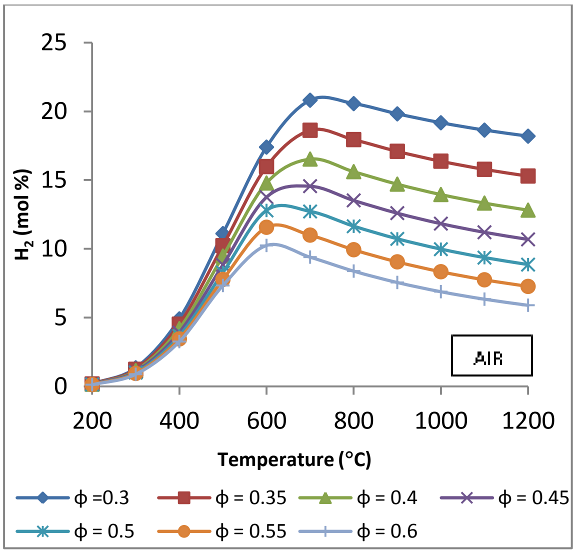
S.No	Major gasification reactions	Chemical equations
1.	Carbon partial Oxidation	$C + 1/2\,O_2 \rightarrow CO$
2.	Carbon oxidation	$C + O_2 \rightarrow CO_2$
3.	Carbon monoxide oxidation	$CO + 1/2\,O_2 \rightarrow CO_2$
4.	Hydrogen oxidation	$H_2 + 1/2\,O_2 \rightarrow H_2O$
5.	Methane partial oxidation	$CH_4 + 1/2\,O_2 \rightarrow CO + 2\,H_2$
6.	Boudouard reaction	$C + CO_2 \rightarrow 2CO$
7.	Primary water gas reaction	$C + H_2O \rightarrow CO + H_2$
8.	Secondary water gas reaction	$C + 2H_2O \rightarrow CO_2 + 2H_2$
9.	Water gas shift reaction	$CO + H_2O \rightarrow CO_2 + H_2$
10.	Hydrogasification	$C + 2H_2 \rightarrow CH_4$
11.	Methanation reactions	$CO + 3H_2 \rightarrow CH_4 + H_2O$ $CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O$ $2C + 2H_2O \rightarrow CH_4 + CO_2$ $2CO + 2H_2 \rightarrow CH_4 + CO_2$
12.	Primary steam reforming	$CH_4 + H_2O \rightarrow CO + 3H_2$
13.	Secondary steam reforming	$CH_4 + 2H_2O \rightarrow CO_2 + 4H_2$
14.	Dry reforming	$CH_4 + CO_2 \rightarrow 2CO + 2H_2$

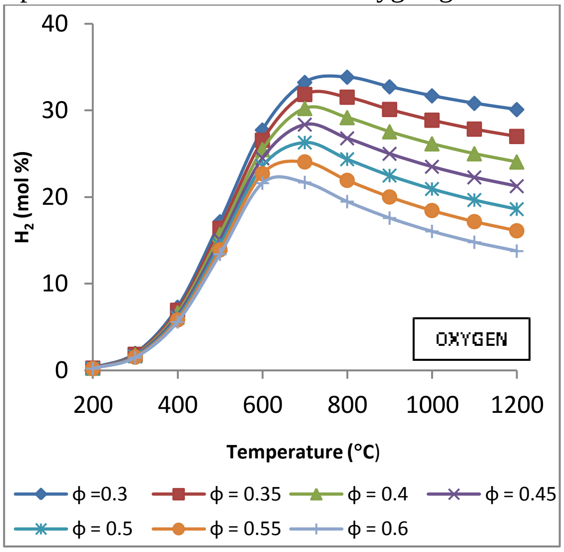
3.2. Effect of equivalence ratio on gas composition

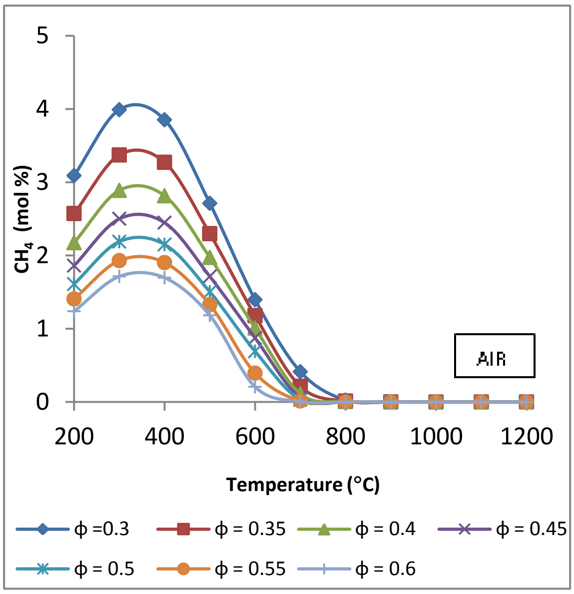
The optimum value of ϕ for biomass gasification varies from 0.2 - 0.4 and selection of ϕ value depend on the application of producer gas [44]. In actual practise change in equivalence ratio alters temperature, which in turn changes equilibrium condition and thus gas composition varies [21] but, in simulations equivalence ratio is varied without altering the temperature. The amount of air supplied is 4.35 times greater in mass than oxygen supply for any fuel. Reduction in gasifying medium requirement decreases size and power consumption of auxiliary components of the gasifier. For both air and oxygen mediums, increase in ϕ value decreases H_2 and CH_4 content for all temperature. Up to 400°C H_2 reduction with the increase in ϕ value is less than 2% for both gasifying mediums. Maximum H_2 reduction of 12.29 and 16.33% are observed in air and oxygen gasification at 1200°C. After 700°C CH_4 is less than 1% for both gasification at all ϕ values except for ϕ=0.3 and 0.35 in oxygen gasification. Equivalence ratio has no effect on CO up to 500°C and at higher temperatures, CO% decreases with increase in ϕ value for both gasifying mediums. CO reduction is justified by combustion occurrence at high ϕ value, improved char burning produces more CO_2 other than combustible gases [45].

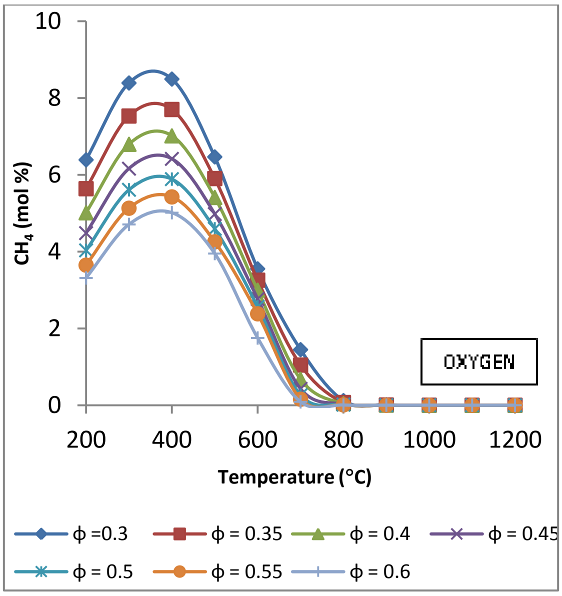
3.3. Gas heating value and cold gas efficiency

Gasifier bed temperature alters both gas composition and gas heating value. For air gasification, maximum HHV of 5.96 MJ/Nm^3 is attained at 700°C for ϕ=0.3. At the corresponding operating condition, LHV=5.53 MJ/Nm^3 and CGE=82.77% are obtained. For oxygen gasification maximum HHV of 9.85 MJ/Nm^3 is attained, corresponding LHV=9.18 MJ/Nm^3 and CGE=83.95% are obtained at 800°C for ϕ=0.3. Heating value fairly remains constant above 700°C although the composition varies. Maximum CCE of 99.89% reached at 800°C and remains constant up to 1200°C for both air and oxygen gasification.









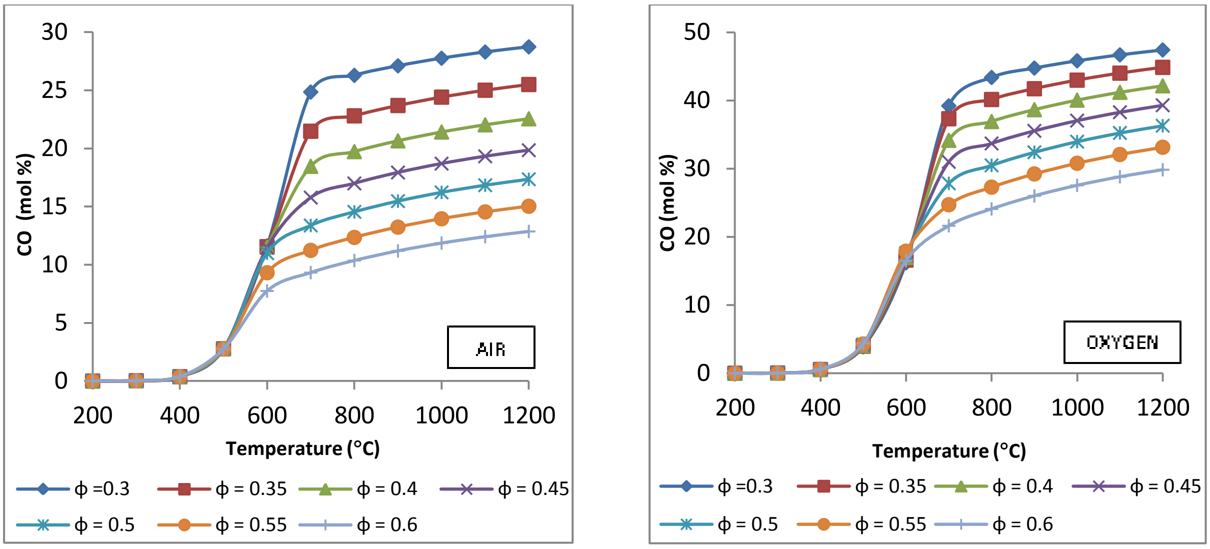


Figure 1. Gas composition of sawdust at different operating conditions for air and oxygen gasification

At a high-temperature heating value of gas decreases due to the reduction of CH_4 and light hydrocarbon production [45]. Combustion is effective at high temperature which improves CO_2 and N_2 production [46]. Carbon conversion increases with the rise in temperature due to oxidation and gasification reactions which in turn increase the gas yield [27, 35, 47]. Calculated HHV, LHV, CCE and CGE are shown in Fig. 2.

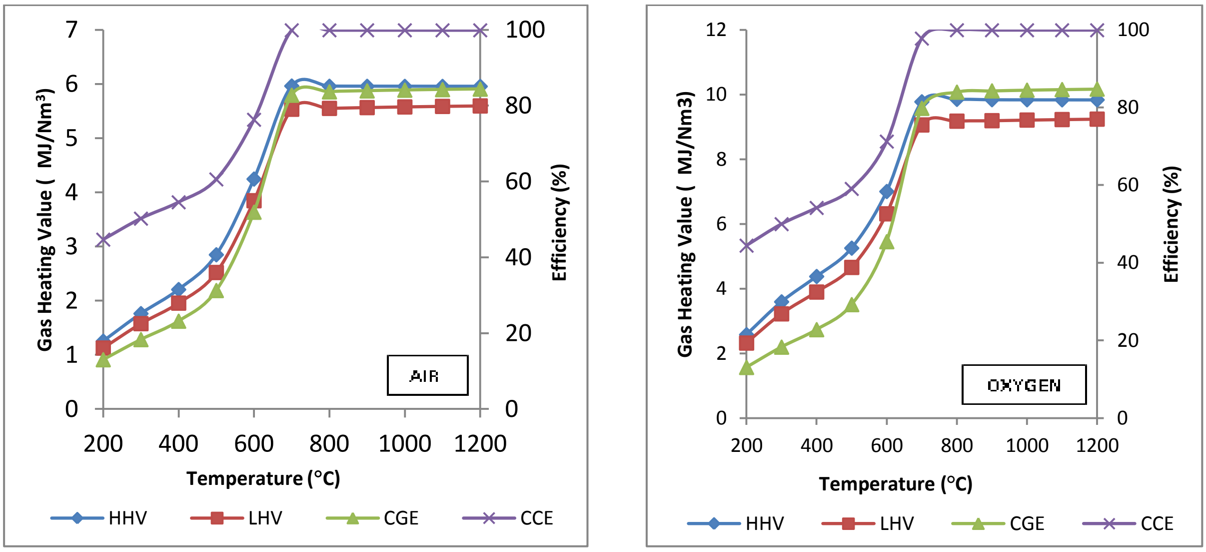


Figure 2. Gas heating value and efficiencies at ϕ = 0.3 for air and oxygen gasification

3.4. Model Validation

Simulation values differ from experimental values due to assumptions present in the equilibrium modelling, in order to accommodate this variation, the accuracy of the simulation has to be analysed. Rice husk air and steam gasification simulation values are compared with experimental values of Karmakar et al [21] and Loha et al [22] respectively. For air gasification, simulation temperature range fixed (600 - 800°C) and incremented by 25°C based on experimental operating condition. The equivalence ratios (ϕ) for simulation are 0.25, 0.35 and 0.45. Comparison of experimental and simulation gas compositions are shown in Fig.3 and importance are given to combustible gas components. For ϕ=0.25 and 0.35, H_2 values are underpredicted for the selected temperature range. The maximum deviation of 0.52% observed at 725°C for ϕ=0.25 and 1.61% at 750°C for ϕ=0.35 respectively. For ϕ=0.45 overprediction of H_2 take place, the maximum deviation of 2.37% occurs at 650°C. For ϕ=0.25 and 0.35 CO value are underpredicted at the initial temperature, a further increase in temperature shows over prediction. Less CO formation in the experiment is due to localised combustion occurrence, favours CO_2 formation. Maximum over prediction deviation of 8.94 and 6.43% occurs at 725 and 700°C respectively, CO under prediction deviations are lower than over prediction. For ϕ=0.45, maximum overprediction of 7.10% occurs at 650°C and the further rise in temperature decreases the deviation. For all the operating conditions CH_4 values are underpredicted, more CH_4 formation takes place in the experiment due to the non-existence of equilibrium condition. The maximum deviation of 1.98, 2.11 and 1.79% occurs at ϕ=0.25, 0.35 and 0.45 respectively with the corresponding temperature of 700, 700 and 600°C. The deviations are estimated by RMS values for each operating condition, average RMS value estimated as 3.59. For rice husk steam gasification, temperature varied from 690 to750°C and steam to biomass ratio 1 - 1.32. Experimental values of gas composition (H_2, CO, CO_2 and CH_4) are compared with simulation values and average RMS value found to be 4.67, shown in Table 3.

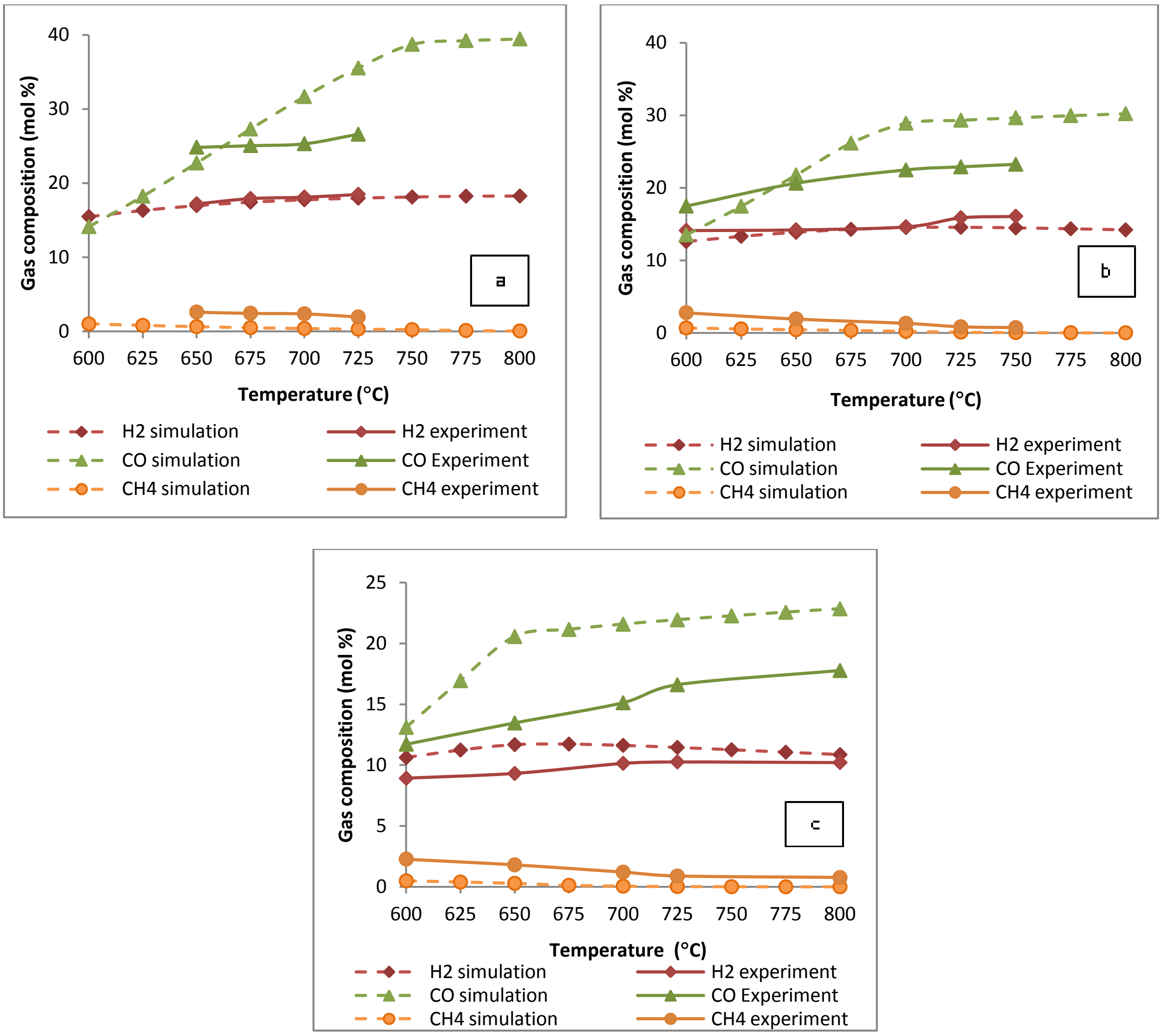


Figure 3. Rice husk air gasification simulation and experimental results [21] (a) ϕ=0.25, (b) ϕ=0.35, (c) ϕ=0.45.

Table 3. Simulation and experimental result of rice husk steam gasification

S. No	Temperature (°C)	S/B ratio	Experimental Value [22]				Simulation Value				RMS
			H_2 (%)	CO (%)	CO_2 (%)	CH_4 (%)	H_2 (%)	CO (%)	CO_2 (%)	CH_4 (%)	
1	690	1.32	50.5	14.3	26.6	8.6	56.06	19.06	24.44	0.43	5.59
2	730	1.32	52.2	16.4	23.5	7.9	55.85	20.81	23.20	0.14	4.82
3	750	1.00	49.5	23.7	21.2	5.6	53.74	26.49	19.59	0.17	3.80
4	750	1.32	52.3	17.75	22.25	7.4	55.65	21.59	22.67	0.08	4.46
										AVG	4.67

4. Conclusions

Air and oxygen gasification simulation of sawdust is carried out to find out the gas composition at the different operating condition. Gas heating values, cold gas efficiency and carbon conversion efficiency are found. H_2, CO, CH_4, CO_2 and H_2O are the main gaseous products formed during oxygen gasification, additionally N_2 present in air gasification. All other gaseous products formation is less than 0.5% in both gasifications. Air gasification reaches 99.8% CCE at 600°C for ϕ=0.5 and oxygen gasification reaches it at 700°C for ϕ=0.35. Air gasification reaches, maximum gas HHV of 5.96 MJ/Nm^3 at 700°C for ϕ=0.3 and oxygen gasification reaches 9.85 MJ/Nm^3 at 800°C for ϕ=0.3. Maximum CGE of 84.37 and 84.73% reached by air and oxygen gasification respectively at 1200°C for ϕ=0.3.

Nomenclature

CCE – Carbon conversion efficiency, [%]
CGE – Cold gas efficiency, [%]
G – Total Gibbs energy, [kJ]
G^0 – Gibbs energy of pure component, [kJ]
HHV – Higher heating value of gas mixture, [kJ Nm^{-3}]
LHV – Lower heating value of gas mixture, [kJ Nm^{-3}]
$LHV_{sawdust}$ – Lower heating value of rice husk, [kJ kg^{-1}]
n_j – Number of moles of component
N – Number of gas components
R – Universal gas constant, [kJ kmol^{-1} K^{-1}]
Y – Gas yield, [Nm^3 kg^{-1}]

Greek symbols

ϕ – Equivalence ratio

Acronyms

RMS – Root mean square

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