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A Simulation Study of Downdraft Gasification of Oil-Palm Fronds using ASPEN PLUS

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Abstract: The use of biomass gasification for conversion of hydrocarbons to permanent fuel gas mainly composed of carbon monoxide and hydrogen, dates back to late 1700. However, the successful design and operation of gasifiers is not an easy task. No clear cut methods of performance prediction of gasifiers is yet available as the thermodynamics of gasifier operation is less understood and highly dependent on the specific biomass feedstock used. In this study, the performance study of downdraft gasification of oil-palm fronds, is carried out making use of ASPEN PLUS process simulator software, to study the effect of operating conditions (zone temperature, operating pressure, air fuel ratio and moisture content) on syngas composition. In this study, the pyrolysis yield is calculated from the ultimate analysis (CHNS test) values of the oil-palm fronds, rather than approximating typical yield distribution for pyrolysis products. The results of the simulation showed better agreement with the syngas composition results of other authors. From the simulation study it is shown that higher mass fraction of CO and CH₄ can be obtained at lower air-fuel ratio and lower pressure (below 5 bars). The mass fraction of CO increases sharply with increase in the oxidation zone temperature, for the temperature range of 500-700°C.

Key words: Biomass, gasification, oil-palm fronds

INTRODUCTION

High prices of conventional sources of energy, like fossil fuels kept on increasing as we face their possible depletion in the near future, while the energy demand of the world is increasing at an alarming rate. Moreover, the high level of environmental pollution caused by increased use of fossil fuels created a greater concern. As a result the world is looking for cheaper, sustainable and environmentally friendly renewable energy sources. One such renewable energy source is biomass waste. Biomass is a solid waste which can be obtained from many sources: living organisms, agriculture waste, forest residues, animal waste and even Municipal Solid Waste (MSW).

The positive features of biomass for energy use include: Low-cost by-product of agriculture or silviculture, low ash and sulfur content and zero increase in the level of CO₂ in the atmosphere, provided that consumption does not exceed annual production (Reed and Das, 1988). The largest source of sustainable and renewable raw material for biomass energy use in Malaysia is the oil palm waste. Today, 3.88 million hectares of land in Malaysia is under oil palm cultivation

(Mahlia *et al.*, 2001). These palm oil plantations yield a staggering amount of harvestable biomass (50 to 70 t/ha/year) and only 10% of this total results in the finished products, namely palm oil and palm kernel oil. The remaining 90% Empty Fruit Bunch (EFB), Kernel Shell, Palm Oil Mill Effluent (POME) and Oil Palm Fronds (OPF) are turned to be biomass waste. While the EFB's are used as steam generation boiler fuel, OPF waste is usually left in the farms to rot for soil nutrition. The present research focuses on OPF, as they are easier to collect, store and to prepare as feedstock.

Biomass gasification is the conversion of hydrocarbons in the presence of air/oxygen to produce synthesis gas, which is a mixture of mostly hydrogen and carbon monoxide. Several processes are involved in the gasification process, that include a great amount of combined phenomena such as homogeneous and heterogeneous chemical reactions, heat, mass and momentum transfers, particle attrition etc. For most gasifier systems these processes can be summarized as follows: (Reed and Das, 1988; De Souza-Santos, 2004).

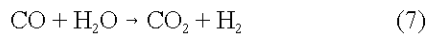
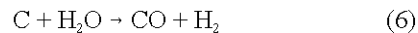
Drying: Liquid water leaves the particle in the form of steam.

Pyrolysis: Biomass + Heat → Charcoal + oil + gases (CO, CO₂, H₂, H₂O, CH₄, C₂H₂, etc).

Combustion: Biomass + Stoichiometric Oxygen → Hot combustion products:



Gasification: Biomass + Limited Oxygen → Fuel gas:



In a real process, all or some of these processes might occur simultaneously, at least for part of the time the processes take place. Though the general discussion and some of the results of this current research might be applicable to other types of gasifiers, the main focus is on downdraft biomass gasifiers. The downdraft biomass gasifier is selected because of the lower level of organic components and its resulting less environmental objection. Moreover, in downdraft gasifiers the acid and tarry distillates of the fuel must pass through a glowing bed of charcoal on their way down and as a result they been converted into permanent gases such as hydrogen, carbon dioxide, carbon monoxide and methane. Therefore, the main advantage of downdraft gasifiers is the possibility of producing a tar-free gas suitable for engine application (Reed and Das, 1988). A significant number of studies were done on different types of gasifiers utilizing various kinds of biomass feedstock with the objective of improving the general understanding of the gasification process and to facilitate performance prediction of the units. Most of the studies demonstrated the phenomenological modeling and simulation of the gasification process (Ruggiero and Manfrida, 1999; Khadse *et al.*, 2006; Mathieu and Dubuisson, 2002; Zainal *et al.*, 2001; Rashidi, 1997; Li *et al.*, 2001; Brown *et al.*, 2006; Ratnadhariya and Channiwala, 2009; Mitta *et al.*, 2006; Jand *et al.*, 2006; Nikoo and Mahinpey, 2008; De Jong *et al.*, 2003; Tinaut *et al.*, 2008; Babu and Sheth, 2006; Giltrap *et al.*, 2003; Sharma, 2008; Xiaodong *et al.*, 2006; Chen *et al.*, 2003) and the rest

focus on experimental investigations (Hsi *et al.*, 2008; Zainal *et al.*, 2002; Lv *et al.*, 2004; Balamohan, 2008). However, no previous study had been carried out for the gasification of oil palm biomass and there is no information available on the kinetic rate of the pyrolysis and gasification of oil palm biomass.

The level of complexity of the models developed range from simpler ones, to more complicated models that use reaction kinetic approaches. The simpler models assume conditions of the ideal, well stirred reactor, with residence time substantially large enough, for all the reactions to reach equilibrium. Such equilibrium models which assume thermodynamic equilibrium and do not consider chemical kinetics and transport rate phenomena are used by a number of authors (Ruggiero and Manfrida, 1999; Khadse *et al.*, 2006; Mathieu and Dubuisson, 2002; Zainal *et al.*, 2001; Rashidi, 1997; Li *et al.*, 2001; Brown *et al.*, 2006), to investigate the effect of operating conditions and feedstock characteristics on output syngas composition. Though the equilibrium model can only estimate the maximum yield which can be achieved ideally, without considering kinetic limitations of the various chemical processes, it is found useful to study the effect of variation of different operating conditions on gasifier performance.

Ratnadhariya and Channiwala (2009) presented three zone equilibrium and kinetic free modeling of biomass gasifier. It offers gas composition, temperature profile and gasifier performance parameters for a downdraft biomass gasifier. First zone of the model considers drying and pyrolysis combined together; second zone is oxidation zone and the third zone is the reduction zone. Each zone has been formulated with: (1) reaction stoichiometry; (2) constituent balance and (3) energy balance along with a number of justifying assumptions-without the needs for kinetic or equilibrium considerations.

In some of the papers, biomass is represented with the general formula CH_xO_y (Ruggiero and Manfrida, 1999; Khadse *et al.*, 2006; Zainal *et al.*, 2001; Ratnadhariya and Channiwala, 2009; Jand *et al.*, 2006; Nikoo and Mahinpey, 2008) where, x and y are the H/C and O/C mole ratio, respectively. A few of the common assumptions made include, char is modeled as pure carbon or graphitic carbon (Ruggiero and Manfrida, 1999; Khadse *et al.*, 2006; Ratnadhariya and Channiwala, 2009; Mitta *et al.*, 2006; Jand *et al.*, 2006; Nikoo and Mahinpey, 2008), 0% char carry over (Zainal *et al.*, 2001; Ratnadhariya and Channiwala, 2009), reactions proceeds adiabatically (Ruggiero and Manfrida, 1999; Khadse *et al.*, 2006; Zainal *et al.*, 2001) particle geometry is considered as spherical (Ratnadhariya and Channiwala, 2009; Nikoo and Mahinpey, 2008; Tinaut *et al.*, 2008). And the major

products of the gasification process are considered to be CO, CH₄, H₂, CO₂ and H₂O (Ruggiero and Manfrida, 1999; Khadse *et al.*, 2006; Ratnadhariya and Channiwala, 2009; Mitta *et al.*, 2006). The method of solutions used to determine the composition of syngas involves application of equations of:

- Atomic balances (species conservation C, O, H, N, S) (Ruggiero and Manfrida, 1999; Khadse *et al.*, 2006; Zainal *et al.*, 2001; Ratnadhariya and Channiwala, 2009; Mitta *et al.*, 2006; Nikoo and Mahinpey, 2008; Tinaut *et al.*, 2008)
- Energy balance (Ruggiero and Manfrida, 1999; Khadse *et al.*, 2006; Zainal *et al.*, 2001; Ratnadhariya and Channiwala, 2009; Nikoo and Mahinpey, 2008; Tinaut *et al.*, 2008)
- Minimization of Gibbs Free Energy (Mathieu and Dubuisson, 2002; Mitta *et al.*, 2006)
- Equilibrium Relations (Ruggiero and Manfrida, 1999; Khadse *et al.*, 2006; Zainal *et al.*, 2001; Rashidi, 1997; Li *et al.*, 2001; Brown *et al.*, 2006)

Mathieu and Dubuisson (2002) used built in equilibrium reactors of ASPEN PLUS process simulator to model a fluidized bed gasifier that uses wood biomass. Jand *et al.* (2006) proposed a method to improve the predicting capability of the equilibrium based calculation, by considering two stage conversion of fast biomass particle devolatilization, followed by much slower and hence often non-equilibrium conversion of methane and char. In this study, the inputs to the equilibrium calculation routines are modified in relation to the latter phenomena based on experimental data. Nikoo and Mahinpey (2008) and De Jong *et al.* (2003) developed kinetic model of fluidized bed gasifiers, using Aspen Plus process simulator for pine saw dust and woody biomasses, respectively.

Tinaut *et al.* (2008) developed a kinetic model of biomass gasification based on the mass and energy conservation Eq. the energy exchange between solid and gaseous phases and the heat transfer by radiation from the solid particles, using the ash-segregation (exposed core model). The kinetic parameters of the gas-gas and solid gas reactions are adopted from literature.

To closely observe the gasification system most authors try to investigate the effect of operating conditions and physical/chemical characteristics of the feedstock on the performance of gasifiers. The common operating conditions and feedstock characteristics considered include: Operating temperature (Ruggiero and Manfrida, 1999; Khadse *et al.*, 2006; Zainal *et al.*, 2001; Jand *et al.*, 2006; Nikoo and Mahinpey, 2008), operating pressure (Ruggiero and Manfrida, 1999; Mathieu and Dubuisson, 2002), Equivalence Ration (ER), (Khadse *et al.*, 2006; Mathieu and Dubuisson, 2002;

Ratnadhariya and Channiwala, 2009; Jand *et al.*, 2006; Nikoo and Mahinpey, 2008; De Jong *et al.*, 2003), particle size (Nikoo and Mahinpey, 2008; Tinaut *et al.*, 2008), air preheat temperature (Mathieu and Dubuisson, 2002; Tinaut *et al.*, 2008), fuel moisture content (Ratnadhariya and Channiwala, 2009; Zainal *et al.*, 2001) and steam to biomass ratio, (Khadse *et al.*, 2006; Mathieu and Dubuisson, 2002; Nikoo and Mahinpey, 2008).

Babu and Sheth (2006) further considered the variation of the char reactivity factor (CRF) along the length of reduction zone of downdraft biomass gasifier, based on the work of Giltrap *et al.* (2003) who considered a constant CRF along the length of the reduction zone. Sharma (2008) considered the fact that char conversion is controlled by kinetic modeling of surface reaction, which is critical to decide optimum reduction zone size and developed a model to identify the critical condition of reaction temperature where all char gets converted into product gases. Moreover, the equations representing the equilibrium and kinetic reaction model have been coupled with energy equation to investigate the effect of variation of length of char bed on the dry gas composition, calorific value, conversion efficiency and power output of a downdraft biomass gasifier.

The major limitation of kinetic modeling of gasification processes is its dependency on knowledge of a very large number of physical and kinetic rate parameters which are usually unique to each biomass and coal type (according to its cellulose, hemicelluloses and lignin constituents). The determination of such parameters is very difficult because of the complexity of the gasification process, which makes development of a phenomenological model that tries to imitate the actual reactions in a mechanistic approach very difficult. For example, if we consider pyrolysis, which is considered to be a precursor to gasification process, it involves solid, liquid and gas phases combined with heat and mass transfer and an impressive amount of heterogeneous reactions (De Souza-Santos, 2004). Consequently studies done on determination of kinetic rate parameters are very rare and for the most part simply non-available (Xiaodong *et al.*, 2006).

Chen *et al.* (2003) addressed the study of gas productivity and the accompanying corrosion of downstream equipment caused by the high content of tar vapor contained in the gas phase, through experimentation. Hsi *et al.* (2008) also experimentally determined the optimum mean Higher Heating Value (HHV) and the corresponding optimum values of operating conditions with a downdraft biomass gasifier using woody biomass. In addition (Zainal *et al.*, 2002; Lv *et al.*, 2004) carried out similar experimental studies with sawdust feedstock on downdraft and fluidized bed gasifiers, respectively.

The main objective of this study includes the study of OPF as a gasification feedstock and prediction of the composition of the produced gas. Equilibrium modeling of downdraft gasification of OPF is carried out, utilizing ASPEN PLUS Version 21.0, to investigate performance and operation characteristics of the process. In addition to studying effect of the various operating conditions on the gasifier performance, the results of the modeling study are also found useful in the selection of suitable air blower for selected feedstock rate and to estimate the maximum temperature of the oxidation zone.

PRELIMINARY CHARACTERIZATION OF THE FEEDSTOCK

Recently studies were made in University Teknologi PETRONAS (UTP) (Balamohan, 2008; Azrul, 2008), on the feasibility of OPF as a feedstock for gasification and on

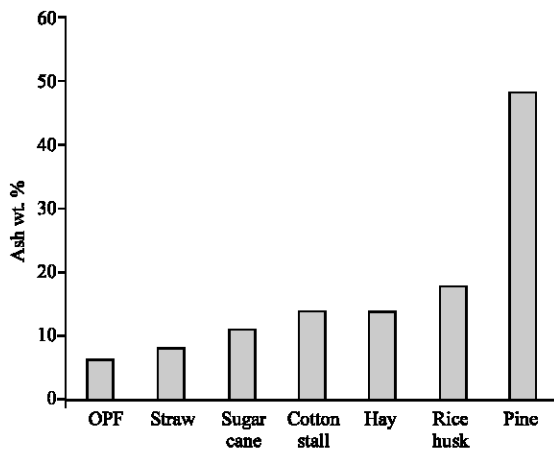


Fig. 1: Comparison of Ash content of OPF with other biomass resources (Balamohan, 2008)

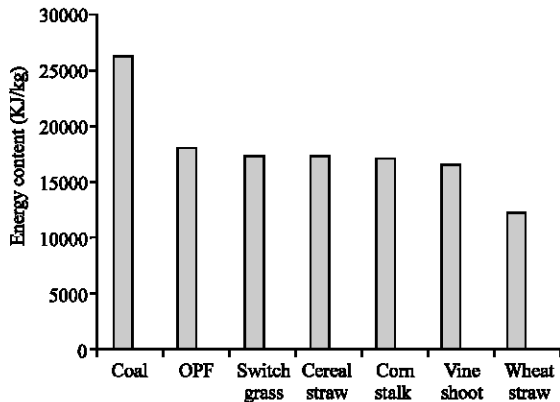


Fig. 2: Comparison of energy content of OPF with other biomass resources (Balamohan, 2008)

preparation of the feedstock. The physical-chemical property of OPF was studied following Ultimate and Proximate Analysis and Calorific Test (Balamohan, 2008; Azrul, 2008). The results of these tests show that OPF has a higher quality in terms of lower ash content, higher calorific value and acceptable moisture content compared to other biomass resources in Fig. 1 and 2.

From the analysis of the physical property of OPF, it was found that OPF has average density of 712.8 kg m⁻³, which is more suitable as compared to other feedstock materials in terms of bulk handling (Balamohan, 2008).

MODEL DEVELOPMENT

Advanced System for Process Engineering (ASPEN) is a software package that gives a complete integrated solution to chemical processes and reactors. The different thermodynamic models of ASPEN include equilibrium and kinetic rate models. As ASPEN PLUS process simulator do not have a built in gasifier model, a number of reactor types defined in ASPEN are used to model each zone of gasification. From the ASPEN PLUS unit operation models, the RStoic reactor model is selected to model the drying zone of the gasification process and the pyrolysis process which involves solid, liquid and gas phases is modeled using the RYield reactor. This model calculates the yield distribution of the products without the need to specify reaction stoichiometry and reaction kinetics, which are less understood for the pyrolysis process. Results of ultimate analysis of the biomass are used to estimate the yield distribution (Nikoo and Mahinpey, 2008). The combustion and reduction zones of gasification are modeled using Gibbs reactor model, assuming equilibrium reaction.

Simulation of the heat and mass balances of a solids process requires a physical properties model suitable for solid components (De Souza-Santos, 2004). Therefore, the special physical property method feature of ASPEN PLUS simulator for non-conventional solids is utilized for defining physical and chemical properties (Table 1) of feedstock material, rather than simply representing the biomass with the general chemical formula such as CH_xO_y (Aspen Plus, 2000a, b). In previous study (Atnaw and Sulaiman, 2009), similar equilibrium modeling study using ASPEN had been carried out assuming typical yield distribution for pyrolysis products (CO, H₂, CO₂, H₂O, CH₄, C₂H₂ etc.). In this study, only the yield of the basic components (H₂O, C, H₂, O₂, N₂ and S) is directly calculated from the ultimate analysis result for the specific feedstock (Table 1), by introducing a Fortran subroutine in the ASPEN PLUS simulation model.

The simulation results of this model showed better agreement with the syngas composition results of other authors (Khadse *et al.*, 2006; Mathieu and Dubuisson,

Table 1: Chemical properties of OPF (AZRUL, 2008)

Analysis	%
Proximate	
Volatile Matter (VM)	53.00
Fixed Carbon (FC)	41.00
Ash	6.00
Ultimate	
C	42.55
H	5.48
N	2.18
S	0.11
O	45.50

*-All values of Proximate and Ultimate analysis are on dry weight basis

Table 2: Initial temperature estimates.

Zone	Temp. (°C)
Drying	300
Pyrolysis	500
Oxidation	850
Reduction	650

2002; Zainal *et al.*, 2001), yet it still needs to be validated with experimental data in the future. The initial estimation of the temperature of the various gasification zones is given in Table 2.

RESULTS AND DISCUSSION

Here, the results obtained from the ASPEN PLUS equilibrium model of downdraft gasification of OPF is presented. The moisture content of the feedstock is considered to be 10% in the simulation and the biomass feed is defined as a non conventional solid in terms of its proximate and ultimate analysis values.

Typical simulation result: Table 3 shows typical simulation results for mass fraction of producer gas for initial input of different operating parameters of the ASPEN PLUS equilibrium model, at the exit of various zones of the gasification unit.

Sensitivity analysis: A sensitivity analysis is done using ASPEN simulator, by varying the values of the operating parameters, pressure, temperature and air fuel ratio, to study their effect on the composition of the producer gas.

Oxidation and reduction zone temperature: The first sensitivity analysis is carried out by varying the oxidation zone temperature for the range of 500-1200°C at 20°C interval. The effect of varying the oxidation zone temperature, on the mass fraction of component gases produced is plotted in Fig. 3. The mass fraction of the component gases CH₄ and CO₂ is found to decrease with increase in temperature inside the oxidation zone, while the mass fraction of CO showed a sharp increase with temperature of the oxidation zone for the range 500-700°C.

Table 3: Typical simulation result

Product	Mass flow (kg h ⁻¹)				
	Feed	Drying	Pyrolysis	Oxidation	Reduction
H ₂ O	0.00	0.63	1.413	4.047	3.074
CO	0.00	0.00	0.00	11.497	9.488
CO ₂	0.00	0.00	0.00	10.341	13.107
C	0.00	0.00	7.752	0.00	0.00
H ₂	0.00	0.00	1.004	0.709	0.782
CH ₄	0.00	0.00	0.00	0.001	0.142
O ₂	0.00	0.00	8.459	0.00	0.00
N ₂	0.00	0.00	0.405	26.64	26.64
S	0.00	0.00	0.037	0.037	0.037
BM	20.00	19.37	0.00	0.00	0.00
ASH	0.00	0.00	0.93	0.93	0.93

The significant rise of composition of CO with temperature is expected as high temperature favors carbon conversion rate, resulting in cleaner producer gas with lower char and tar condensate and higher calorific value (Lijun *et al.*, 2008). The values of the results obtained in this simulation are not directly comparable with values from literature, as the type of feedstock, the type of gasifier unit and some of the operating conditions considered are different. However, an acceptable agreement is observed in the shape and trend of the curves. For instance, the mole fraction of CO increased from 2.5 - 24% for temperature range of 500-700°C, in the work of (Khadse *et al.*, 2006), for updraft gasification of sawdust. The current simulation revealed that the mole fraction of CO is predicted to increase comparably from 5-18% for the same range of temperature. Also the mole fraction of H₂ increased from 9-16% for the case of (Khadse *et al.*, 2006) while it is predicted to increase from 10-19% in the present simulation study for OPF gasification. Comparable trend is observed for variation in the reduction zone temperature over the temperature range of 400-1000°C in Fig. 4.

Pressure: Sensitivity analysis carried out with respect to operating pressure of the oxidation zone (Fig. 5) showed that, the mass fraction of CO, H₂ and CH₄ falls rapidly as the pressure inside the oxidation zone exceeds a value of 5 bars. This prediction is in agreement with literature as the yield of CO and H₂ is known to decrease with pressure while that of CO₂ increases (Higman and Van der Burgt, 2008).

Air fuel ratio: The simulation results also showed that the mass fraction of the fuel components CO and CH₄ are higher at lower air fuel ratio. A slight increase in the mass fraction of CO₂ is shown as the Air-Fuel ratio increased up to 80% in Fig. 6. Mathieu and Dubuisson (2002) also obtained similar trends for CO and H₂O by carrying out ASPEN equilibrium model simulation for fluidized bed gasifiers and performing sensitivity analysis with respect to air fuel ratio. As it is obvious the mass fraction of N₂ in syngas increases with AFR.

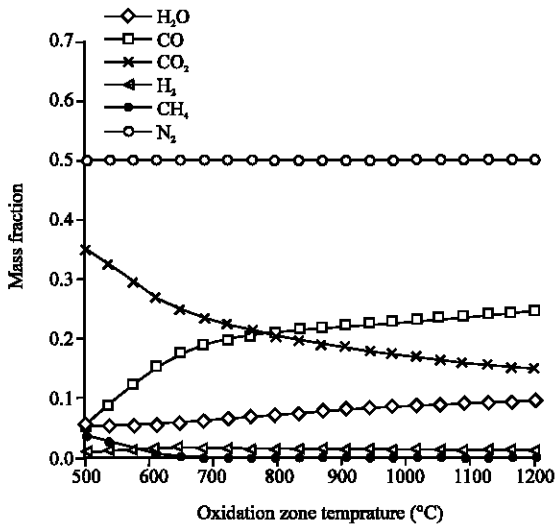


Fig. 3: Variation of component mass fraction with oxidation zone temperature

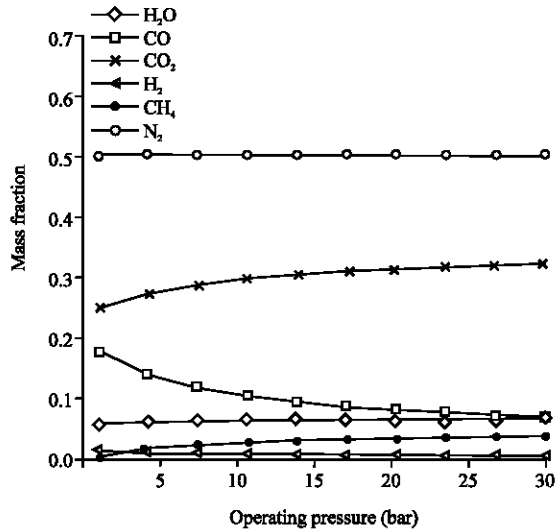


Fig. 5: Variation of component mass fraction with operating pressure

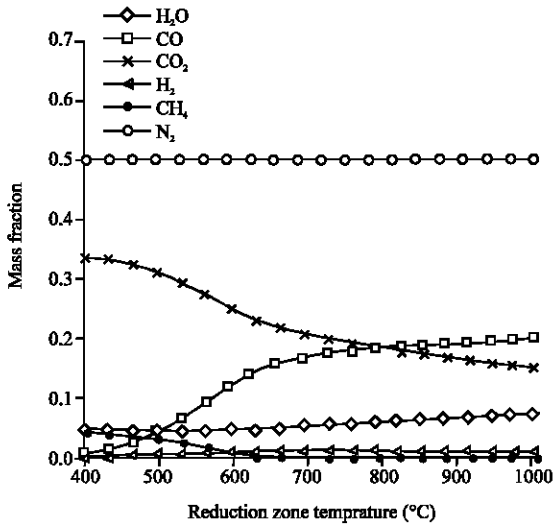


Fig. 4: Variation of component mass fraction with reduction zone temperature

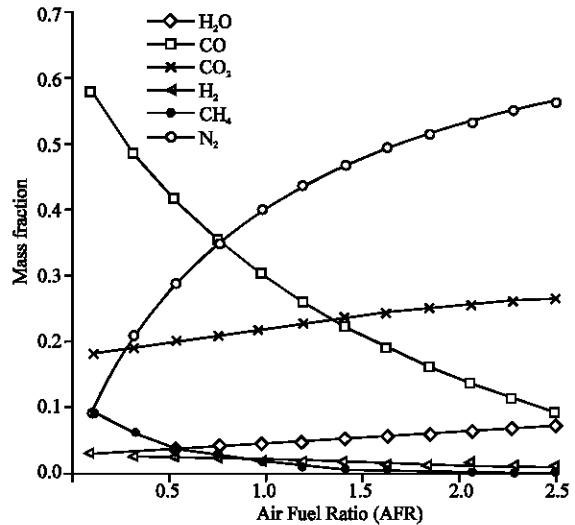


Fig. 6: Variation of component mass fraction with air-fuel ratio at pressure of 1.05 bar and oxidation zone temperature of 850°C

Moisture content: A prediction of equilibrium composition is done for the range of values of moisture content (MC) (5 to 20%) of the feedstock. This analysis revealed that the mass fraction of CO decreases while that of CO₂ and H₂O slightly increases and the mass fraction of N₂ and H₂ remains constant with increase in MC (Fig. 7). A similar trend is observed in the work of Zainal *et al.* (2001) that uses equilibrium modeling of a downdraft biomass gasifier operating on sawdust feedstock and the prediction of Ratnadhariya and Channiwala (2009) with equilibrium and kinetic free model. The value of the mole fraction CO decreases from 28-20%

and 19-17% for the case of Zainal *et al.* (2001) and Ratnadhariya and Channiwala, (2009), respectively, for the increase in MC from 0 to 20%. The result of the present simulation using ASPEN for the same range of MC found to vary from 22-15% (mole fraction basis), showing a similar trend and closer range of values. Also the mole fraction of H₂, varies from 20-25% and 23-20% in the work of Zainal *et al.* (2001) and Ratnadhariya and Channiwala (2009), respectively for the range of MC values of 0-20%. Whereas, the simulation result for the gasification of OPF showed 17-15% decrease in mole fraction of H₂.

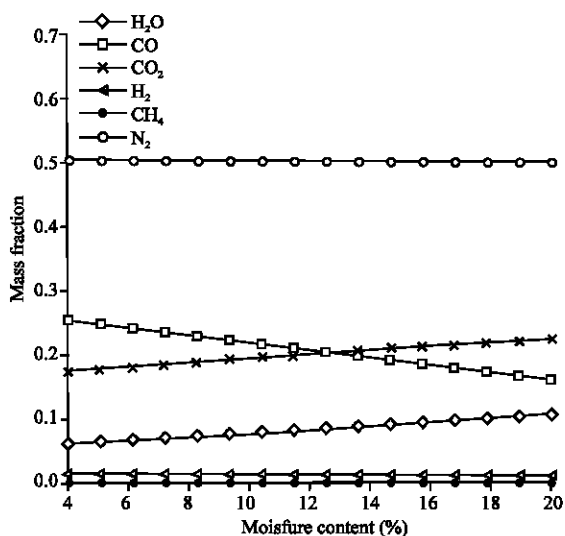


Fig. 7: Variation of component mass fraction with moisture content

CONCLUSIONS

In this study, a downdraft biomass gasification model is developed using the built-in reactor models of ASPEN PLUS Version 21.0, process simulator assuming equilibrium reactions. This model allowed the study of the effect of operating pressure, temperature, air fuel ratio and moisture content on the product gas composition in terms of mass fraction. From the simulation results it is found that the mass fractions of the major fuel components of the product gas; CO, H₂ and CH₄ are higher at lower air-fuel ratio, higher oxidation temperature and lower operating pressure values below 5 bars. In addition to helping in the performance prediction and study of the gasification process at different operating conditions, the simulation results helped to predict the maximum temperature of the oxidation zone as well as the flow rate and pressure requirement of a blower to be used with such units at design stage. In the future it is recommended to further investigate the gasification processes using more comprehensive models and to validate the models through experiment, making use of the specific feed stock material.

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