

# Simulation of Air-Gasification of Wood Wastes Using Aspen Plus

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**Abstract-** A thermodynamic equilibrium model for air-gasification of wood wastes in fixed-bed downdraft gasifier was developed using Aspen (Advanced System for Process Engineering) Plus based on minimisation of Gibbs free energy. The synthesis gas (syngas) composition predicted by the model was found to be in fair agreement with measured syngas composition from experiments with similar gasifier type and biomass. The validated model was used to carry out sensitivity analysis to study the effect of gasifier temperatures, air-fuel ratios and wood waste moisture levels on syngas quality (composition and energy content). The various parameters investigated were observed to affect the syngas quality significantly.

**Keywords** Biomass, equilibrium model, gasification, syngas, wood wastes.

## 1. Introduction

Biomass is a salient energy resource that is readily available and could be harnessed via gasification technology for clean energy generation. Biomass gasification is a continuous sub-stoichiometric process, which converts biomass into syngas (an energy carrier, which can be used to generate energy and produce vital chemicals). The gasification process comprises of drying, pyrolysis (decomposition) as well as oxidation and reduction of the pyrolysis products. Computer software packages are now been used to develop models to study gasification processes as this is more cost effective than carrying out actual experiments as well as providing answers to questions that can hardly be answered by experiments. Among the many available software packages is Aspen Plus, which is a chemical process software that is well suited to build a thermodynamic equilibrium model (TEM) for simulation of gasification processes.

Several authors have deployed Aspen Plus to study biomass gasification processes. Mansaray et al [1, 2, 3]

modelled a fluidized bed gasifier to study rice husk gasification using two separate approaches: equilibrium approach where the hydrodynamic conditions were ignored and a second approach where the hydrodynamic conditions were accounted for. The models predicted syngas composition and syngas HHV that agreed reasonably well with experimental results. Mathieu and Dubuisson [4] modelled a fluidized bed gasifier based on minimisation of Gibbs free energy to study wood gasification. The gasification process was broken into pyrolysis, oxidation and reduction. Sensitivity analysis conducted revealed an optimal air temperature value beyond, which air preheating is inefficient, and a maximum oxygen factor. Mitta et al [5] modelled a fluidized bed gasifier based on minimisation of Gibbs free energy to study gasification of tyre with air and steam as oxidants. The gasification process was sectionalized into drying, pyrolysis and gasification/oxidation. The Model predicted syngas composition with good accuracy when compared with experimental results. Nikoo and Mahinpey [6] appraised the performance of a fluidized bed gasifier using air as oxidant under steady state, simultaneous hydrodynamic and kinetic conditions. Several in-built Aspen Plus reactors and external

FORTRAN codes were utilized to model the gasification process. Model results revealed that  $H_2$  concentrations increased with temperature;  $CO_2$  and carbon conversion efficiency (CCE) increased as equivalence ratio increases; then as the steam/biomass ratio increased,  $H_2$  and  $CO$  increased while  $CO_2$  and CCE decreased respectively. Hannula and Kurkela [7] modelled a fluidized bed gasifier under high pressure using several blocks and FORTRAN subroutines to study biomass gasification of different wood wastes. The model was found suitable for evaluating the gasification of pinewood sawdust and chips, eucalyptus chips and forest wastes, but not for pinewood bark and wheat straw. Ramzan et al [8] developed a steady-state model based on minimization of Gibbs free energy to investigate the gasification of municipal solid, food and poultry wastes. Model results revealed that molar fractions of  $CO$  and  $H_2$  increased with increase in temperature, but decreased as the equivalence ratio increased, thereby decreasing the cold gas efficiency. Concentrations of  $H_2$  and  $CO$ , syngas HHV and CGE were highest for food waste gasification and lowest for poultry waste gasification. Mavukwana et al [9] studied sugarcane bagasse gasification using Aspen Plus. The model predicted syngas composition that was in good agreement with experimental results published in literature. Kuo et al [10] developed a thermodynamic equilibrium model of a fixed-bed downdraft gasifier to study the gasification of bamboo (both in its raw and torrefied forms). They discovered that equivalence ratio as well as steam-biomass ratio had significant effects on the produced syngas composition. Chen et al [11] modelled fixed bed reactors to study municipal solid waste (MSW) gasification. They observed that variations in temperatures and equivalence ratio had slight effects on syngas composition, syngas LHV and gasifier conversion efficiency.

Other authors who have also utilized Aspen Plus to model biomass gasification processes include [12] who developed an equilibrium model for a sawdust-fired downdraft gasifier as well as [13] with equilibrium and kinetic free modelling. Some researchers have also developed models for coal, biomass and/or wastes co-gasification processes using Aspen Plus. These researchers include [14] who built a model of an integrated gasification combined cycle (IGCC) using biomass as feedstock for electricity generation. Yan and Rudolph [15] model a sectionalized fluidized-bed gasifier for coal gasification. Sudiro et al [16] modelled pet-coke gasification for natural gas synthesis. Paviet et al [17] developed a simplistic two-step equilibrium model for wood gasification. Doherty et al [18,19] modelled biomass gasification processes in a circulating fluidized bed gasifier to study how variations in the equivalence ratio, temperature, degree of air pre-heating, moisture content of biomass and steam/biomass ratio will affect syngas composition and energy content as well as gasification efficiency. Michailos and Zabaniotou [20] modelled a bubbling fluidised bed gasifier, based on a minimization of Gibbs free energy and reaction kinetics, to study olive kernel gasification using air as oxidant. Kumar et al [21] investigated the gasification of corn stover and distiller grains and reported that the model predicted the syngas yield and composition with fair accuracy.

This study is a part of a project aimed at building local capacity in gasification technology development and deployment in Sub-Sahara Africa, especially in Nigeria. A pilot biomass gasification system, comprising a fixed bed downdraft gasifier and a syngas cleaning unit (made up of cyclone separator, syngas cooler and coarse filter), was developed at the University of Benin, Nigeria. The design and development of the downdraft gasifier system was presented in [22]. Previous work on the project involved conducting gasification experiments with the system, using wood wastes as feedstock and atmospheric air as oxidant, to assess its performance in terms of syngas yield, composition, and energy content, biomass consumption rate as well as carbon conversion efficiency. This current study deals with the modelling and simulation of air-gasification of wood wastes in the downdraft gasifier system using Aspen Plus software to investigate how variations in operating parameters (gasifier temperature, air-fuel ratio and biomass moisture levels) would affect quality of the produced syngas.

## 2. Materials and Methods

### 2.1. Process Model Simulator

Aspen Plus was utilized in the study to model and simulate air-gasification process of mixed wood wastes in a downdraft gasifier. The wood waste gasification process was modelled based on mass - energy balance and chemical equilibrium for the entire process, minimization of Gibbs free energy and ample residence time for all chemical reactions to attain equilibrium. The following sequential steps were employed in building the Aspen Plus model:

- a) Specify stream class,
- b) Select property method,
- c) Specify system components and identify conventional and non-conventional components,
- d) Define the process flowsheet (with unit operation blocks, materials and energy streams),
- e) Specify feed streams,
- f) Specify unit operation blocks.

### 2.2. Assumption

In the study, the following assumptions were made:

- a) Steady state, kinetic free and isothermal conditions,
- b) Chemical reactions occur at equilibrium,
- c) All elements partake in chemical reactions and contact one another uniformly,
- d) Ideal condition for all gases, and any available sulphur converts to  $H_2S$ ,
- e) Tars in syngas are negligible,
- f) Char contains just carbon and ash.

### 2.3. Physical property method

Selecting the appropriate proper property method is important as it is crucial to the outcomes from the simulation.

From reviewed literature, different property methods were chosen to estimate physical properties of conventional components. Table 1 presents the property methods selected by various researchers. Hence, Peng Robinson (PR), Peng Robinson with Boston-Mathias alpha function (PR-BM) and Redlich Kwong-Soave with Boston-Mathias alpha function (RKS-BM) were selected and used respectively as the physical

property method in this study. The results from the use of each property method were validated with results from [41] and previous experimental study by the authors. The property method whose outcomes were in better agreement with the experimental results was selected for estimation of all physical properties of conventional components for the sensitivity analysis in this study.

**Table 1.** Physical property methods chosen by several researchers

Redlich Kwong Soave with Boston-Mathias alpha function (RKS-BM)	Peng Robinson with Boston-Mathias alpha function (PR-BM)	Peng Robinson (PR)	IDEAL	Method not indicated
[17,23,24,25,26,27]	[5,8,12,13,28,29,30]	[10,31,32,33]	[34]	[1,2,3,4,6,7,9,18,19,35,36,37,38,39,40]

HCOALGEN and DCOALIGT were selected to define the enthalpy and density of wood waste and ash respectively, as they are non-conventional components. The stream class was defined as MCINCPSD, which encompasses mixed, conventional solids and nonconventional solids sub-streams. Gases were considered as mixed sub-streams, char as conventional solid sub-stream, wood waste and ash as nonconventional solid sub-streams.

*2.4. Model description and sequence*

The gasification process was modelled in three stages using several of Aspen Plus blocks. The first stage involved

reducing the wood waste moisture content before feeding it into the gasifier. The second stage entailed the decomposition of the wood waste into volatile conventional components and char. A FORTRAN statement in a calculator block was used to specify the yield distribution for this stage. The third stage models the partial oxidation and reduction by minimizing Gibbs free energy. The fourth stage models the separation of ash from the produced syngas. Six (6) blocks in Aspen Plus were deployed to model the downdraft gasifier. These blocks are described in Table 2 while Table 3 presents the data fed into the model.

**Table 2.** Description of Aspen Plus blocks used for the model

Aspen Plus block ID	Block ID in model	Description
RStoic	Dry-REAC	Reduces wood waste moisture content
Flash 2	DRY- FLSH	Separates water vapour from dry wood waste
RYield	DECOMP.	Yield reactor- breaks down wood waste into conventional constituents (using a FORTRAN sub-routine)
RGibbs	GASIFY	Handles multiphase equilibrium and computes syngas composition by reducing Gibbs free energy
Mixer	MIXER	Mix conventional components from yield reactor with air
SSplit	CYCLONE	Removes ash from syngas by defining split fractions.

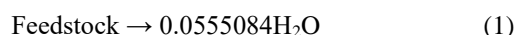
**Table 3.** Data fed into the developed Aspen Plus model

Ultimate analysis (wt. % dry basis)		Proximate analysis (wt. % dry basis)	
Carbon	57.54	Volatile matter	87.55
Hydrogen	5.21	Fixed carbon	9.77
Oxygen	37.10	Ash	2.68
Nitrogen	0.11		
Sulphur	0.04		
Ash	2.68		
Mass flow of wood wastes (kg/h)		1.0	
Moisture content (after pre-drying) wt. %		7.52	
LHV (dry basis) MJ/kg		19.85	
Mass flow of air (kg/h)		1.7	

Figure 1 and Fig. 2 describe the ASPEN Plus flowchart and simulation flowsheet (indicating its computation sequence) for the downdraft gasifier. The wood waste was specified as a nonconventional component and defined using its ultimate and proximate analyses. Table 4 presents the information used to describe the wood waste.

**2.4.1. Drying**

Aspen Plus stoichiometry reactor (“RStoic”) was used to model the drying stage. A FORTRAN statement in the calculator block (DRY CALCULATOR) was utilized to control the drying. RStoic converts part of the feedstock into water according to the reaction represented as



In this stage, the water in the wood waste was partially evaporated and removed using a flash separator block,

by specifying their split fractions. The dried wood waste is fed into the next stage for decomposition.

**2.4.2. Decomposition**

Decomposition is a crucial stage in biomass gasification modelling. In this stage biomass, being non-conventional, is broken down into its constituent elements (C, H<sub>2</sub>, O<sub>2</sub>, N<sub>2</sub>, S, H<sub>2</sub>O and ash; which are conventional) according to its ultimate analysis in a yield reactor (“RYield”). A FORTRAN statement in the calculator block (BRKDOWN CALCULATOR) specified the yield distribution of the wood waste into its constituents. The statement specified the mass flowrates of the constituent elements in the outlet stream (DECPROD). The decomposed constituents are mixed with air in a mixer before being fed into the next stage for gasification.

**Table 4.** Characteristics of mixed wood wastes

Ultimate analysis (%wt. dry basis)		Proximate analysis (%wt. dry basis)	
Carbon	57.54	Volatile Matter	87.55
Hydrogen	5.21	Fixed Carbon	9.77
Oxygen	37.10	Ash	2.68
Nitrogen	0.11	Moisture content (before drying)	25%
Sulphur	0.04	Moisture content (after drying)	5%

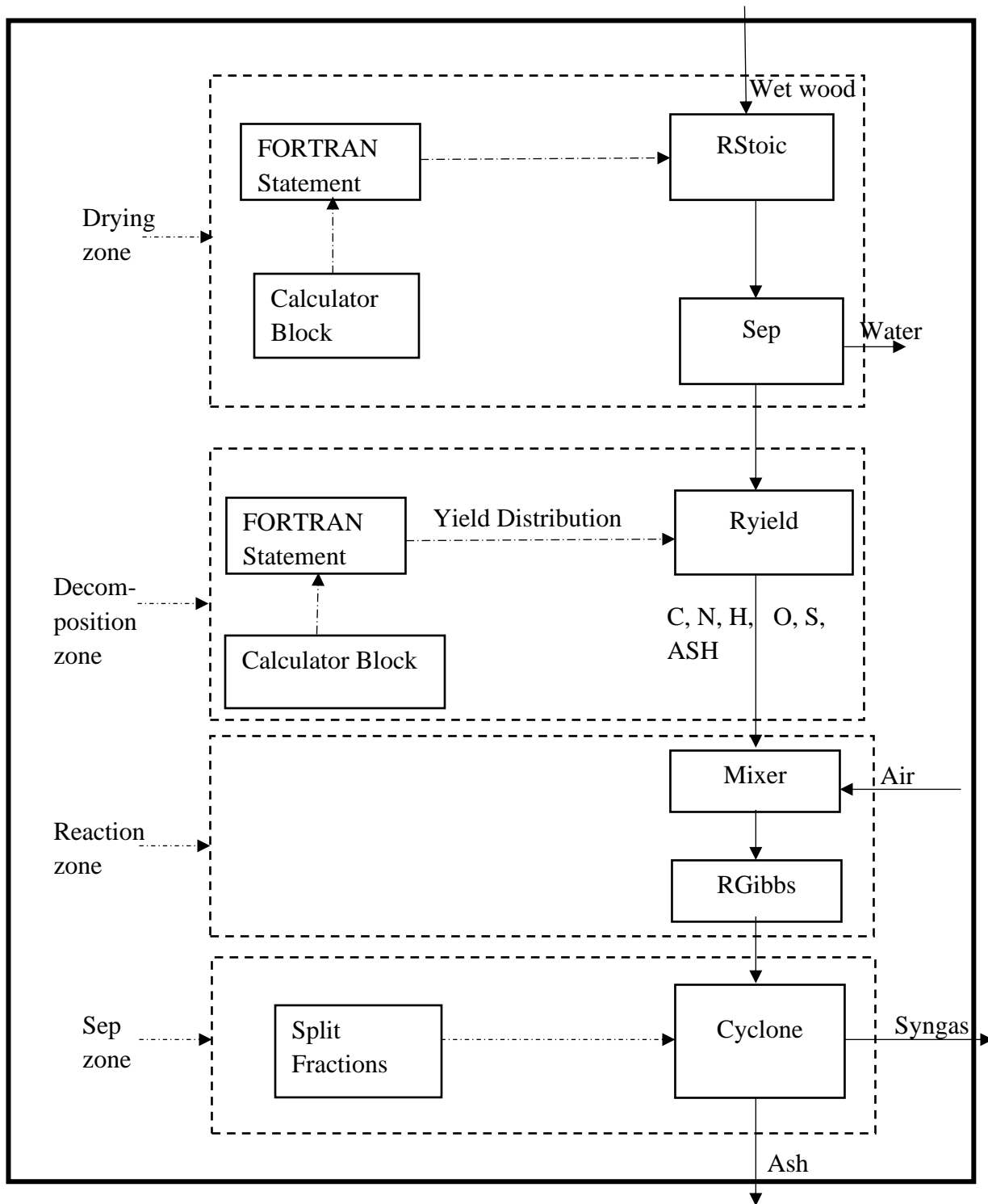
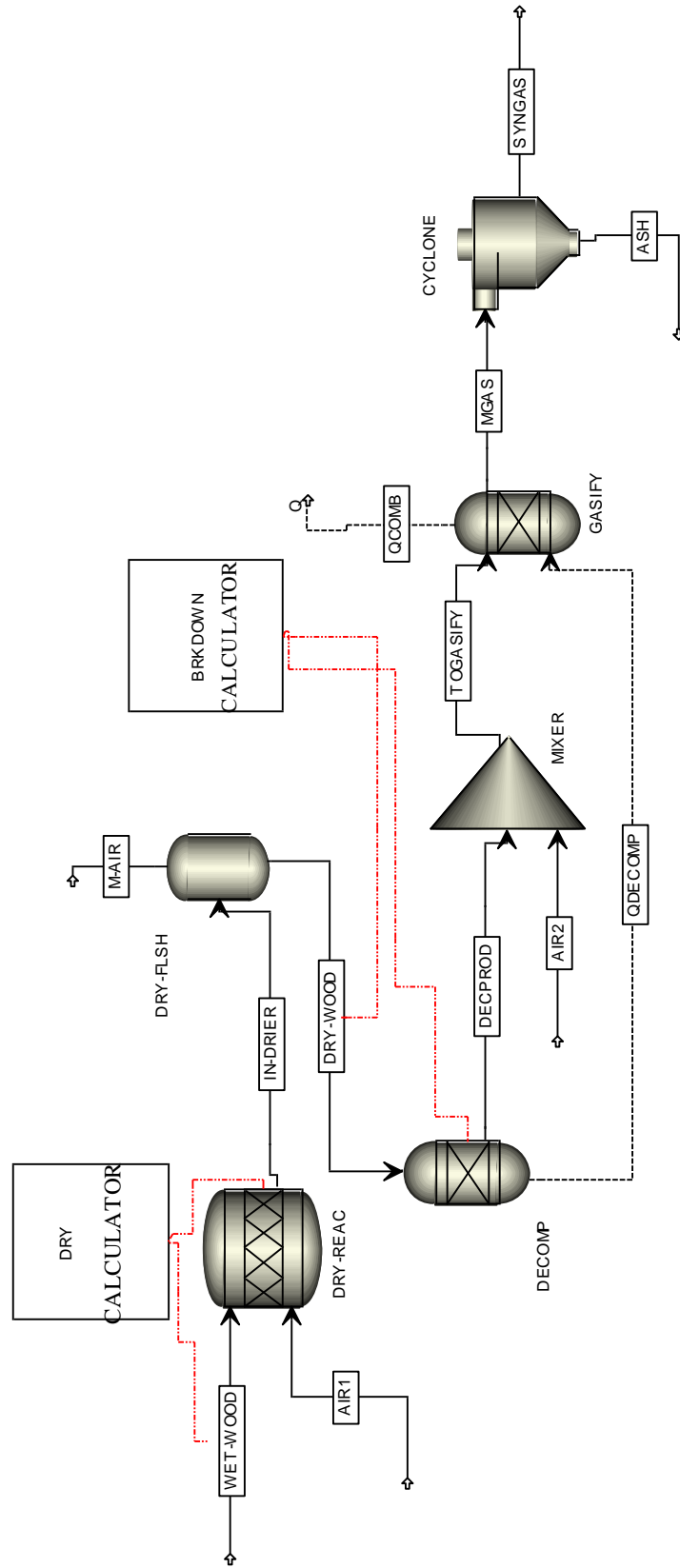


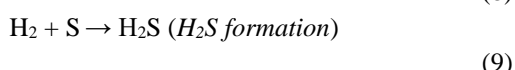
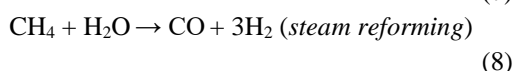
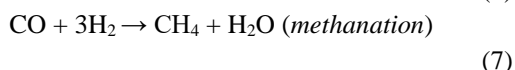
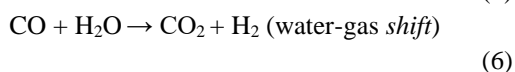
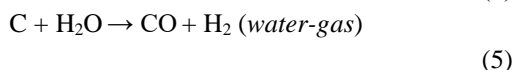
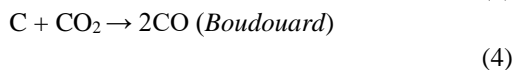
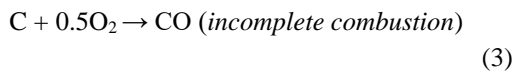
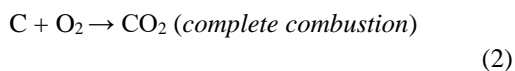
Fig. 1. Aspen Plus simulation flowchart for the downdraft gasifier



**Fig. 2.** Aspen Plus simulation flowsheet for the downdraft gasifier

2.4.3. Oxidation and Reduction

RGibbs reactor is a rigorous reactor for multiphase chemical equilibrium based on minimization of Gibbs free energy. The reactor was selected to model the partial oxidation and reduction processes. As a nonconventional component, it is impossible to calculate Gibbs free energy of wood waste. Hence, the need to break it down into its constituents elements before feeding into the RGibbs reactor (GASIFY). Air is mixed with the feedstock constituents before feeding into the RGibbs reactor, where the mixture is partially oxidised and reduced. The RGibbs reactor computes the syngas composition by minimising Gibbs free energy and assuming complete equilibrium for chemical reactions. Carbon exits partially as gas (which partakes in reactions) and as solid. The major reactions taking place are delineated in Eq. (2) – Eq. (9) [19, 21, 42].



The whole sulphur in the wood waste reacts with H<sub>2</sub> to yield H<sub>2</sub>S. The wood waste has low sulphur content hence, inaccuracies of this assumption are negligible. Ash separation from the syngas was modeled with a unit operation block SSplit (CYCLONE). The stream leaving the RGibbs reactor (MGAS) enters SSplit block, where syngas in the stream ‘SYNGAS’ is separated from ash in the stream ‘ASH’ according to specified split fractions.

2.5. Model Validation

The model results were validated with results from previous experimental study by the authors and [41]. Wei et al [41] conducted experiments on a pilot downdraft biomass gasification system installed at the Department of Agricultural and Biological Engineering, Mississippi State University, Mississippi, USA. The gasification system uses wood chips as feedstock and ambient air as gasifying agent. The ultimate and

proximate analyses of the wood chips are highlighted in Table 5.

**Table 5.** Characteristics of wood chips from [41]

Ultimate analysis (wt. % dry basis)		Proximate analysis (wt. % dry basis)	
Carbon	49.817	Volatile matter	79.850
Hydrogen	5.556	Fixed carbon	19.031
Oxygen	43.425	Ash	1.119
Nitrogen	0.078		
Sulphur	0.005		
Ash	1.119		
Moisture content (as received) wt. %		25.00	
Moisture content (after pre-drying) wt. %		8.91	
LHV (dry basis) MJ/kg		18.58	
Bulk density		222.15	

2.6. Model Application

The developed model was used to investigate how variations in temperature, air-fuel ratio (AFR) and biomass moisture levels would affect syngas quality (in terms of composition and LHV). The lower heating value of syngas depends on the content of the combustible gases (CO, H<sub>2</sub> and CH<sub>4</sub>) in the syngas and could be computed using Eq. (10) [42].

$$LHV_g = (x_{CO} * LHV_{CO}) + (x_{H_2} * LHV_{H_2}) + (x_{CO_2} * LHV_{CO_2}) \tag{10}$$

Where, x = mole fraction of gas constituents, LHV<sub>g</sub> = lower heating value of syngas

3. Results and Discussion

Table 6 compared the experimental results from [41] with the model predicted results.

**Table 6.** Comparison of experimental results from [41] and Aspen Plus model predictions

Syngas composition	Wei <i>et al.</i> 2009	Aspen Plus model		
		PR-BM	PR	RKS-BM
H <sub>2</sub>	18.32	25.25	24.12	19.94
CO	20.93	16.12	13.0	20.13
CO <sub>2</sub>	12.87	15.65	17.32	13.49
N <sub>2</sub>	44.79	42.97	45.45	45.58
CH <sub>4</sub>	3.09	0.00014	0.0000566	0.000151

Table 7 presents comparison of model results with experimental results from previous experimental study by the authors.

**Table 7.** Comparison of experimental results and model results from this study.

Syngas composition	Experi-mental results	Model results		
		PR-BM	PR	RKS-BM
H <sub>2</sub>	16.64	20.32	19.87	16.89
CO	28.15	24.97	22.59	28.65
CO <sub>2</sub>	6.19	8.72	4.77	7.04
N <sub>2</sub>	46.02	45.80	44.80	45.98
CH <sub>4</sub>	2.54	0.000552	0.000033	0.00025

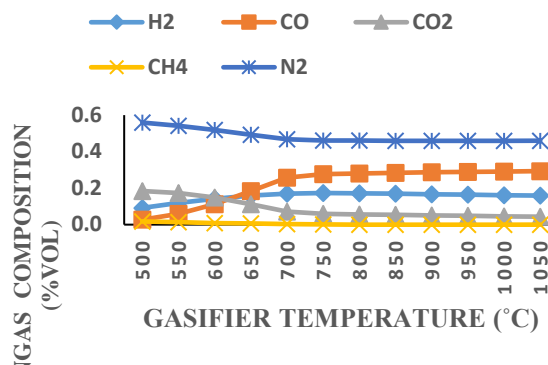
It can be observed from Tables 6 and 7 that syngas composition predicted by the model with RKS-BM as physical property method was in better agreement with syngas composition measured by [41] and in this project. This could be adduced to the suitability of the RKS-BM property method to handle non-polar or mildly polar mixtures like light gases such as CO<sub>2</sub>, H<sub>2</sub>S and H<sub>2</sub>, and the parameter alpha makes the property package able to correlate pure components' vapour pressure at high temperatures. Tables 6 and 7 also reveal that the model with RKS-BM predicted molar fractions of H<sub>2</sub>, CO, N<sub>2</sub> and CO<sub>2</sub> with reasonable accuracy. However, the concentrations of methane (CH<sub>4</sub>) were understated, which is quite prevalent in equilibrium modelling [43, 44]. This underestimation can be adduced to the presence of tars in

syngas from real gasification experiments, which are negligible in equilibrium models, and much more hydrocarbons than model prediction [44, 45, 46]. The under-prediction of CH<sub>4</sub> content resulted in lower syngas LHV from the model than from experimental results.

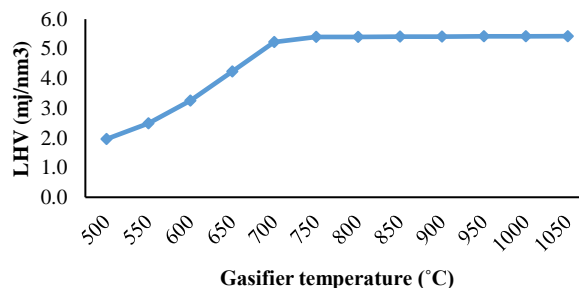
### 3.1. Sensitivity Analysis with the Aspen Plus Model

#### 3.1.1. Effect of gasifier temperature

Fig. 3 and Fig. 4 show the influence of gasifier temperature on syngas composition and LHV.



**Fig. 3.** Variation of syngas composition with gasifier temperature



**Fig. 4.** Variation of syngas LHV with gasifier temperature

The gasifier temperature was varied from 500 - 1050°C, at an increment of 50°C. Figure 3 indicates that as the gasifier temperature increases from 500°C to 1050°C, H<sub>2</sub> content increased initially and attained a maximum value at 750°C, then decreased continuously until 1050°C. CO content increased with increase in temperature until 1050°C, while CO<sub>2</sub> and CH<sub>4</sub> concentrations decreased with increase in temperature. N<sub>2</sub> decreased with increase in temperature until 900°C and then maintained a constant level until 1050°C. Ramzan et al, Puig-Arnavat et al, and Son et al[8, 45, 47] reported similar variations. These trends results from the various reactions taking place during the gasification process. At low temperatures, a huge percentage of carbon in the feedstock is unutilized resulting in low syngas yield. However, as temperature increases more carbon is oxidized, increasing its conversion rate into CO according to Boudouard



reaction (Eq. 4) while methane is converted to hydrogen by steam reforming reaction (Eq. 8). These result in increase in the gasifier temperature, which favours the production of H<sub>2</sub> and CO, consequently improving the energy content of the syngas. Fig. 4 indicates that the syngas LHV experienced a sharp rise as gasifier temperature increased from 500°C to 900°C. It however, experienced slight increase until 1050°C. Ramzan et al, and Puig-Arnavat et al [8, 45] reported similar variations.

### 2.3.2. Effect of air-fuel ratio

Air-fuel ratio is a ratio of the mass of air required to completely combust a given mass of fuel. It has a strong influence on syngas quality. In this study, the air-fuel ratio was varied from 1.35 to 1.89 at 950°C. Figure 5 and Fig. 6 show the influence of air-fuel ratio on syngas composition and LHV. Figure 5 shows that increase in air-fuel ratio increases the content of CO<sub>2</sub> and N<sub>2</sub> but decreases that of H<sub>2</sub>, CH<sub>4</sub> and CO. This is because the process shift towards combustion with increasing air-fuel ratio. Ramzan et al, Puig-Arnavat et al, and Rupesh et al [8, 45, 48] reported similar variations. As observed from Fig. 6 syngas LHV constantly dropped in value with increase in air-fuel ratio. This is as an obvious consequence of decrease in mole fractions of the combustible gases (H<sub>2</sub>, CH<sub>4</sub> and CO) as the air-fuel ratio increases. Devi et al [49] reported that high air-fuel ratio decreases the content of H<sub>2</sub> and CO as well as the LHV, while CO<sub>2</sub> content would increase.

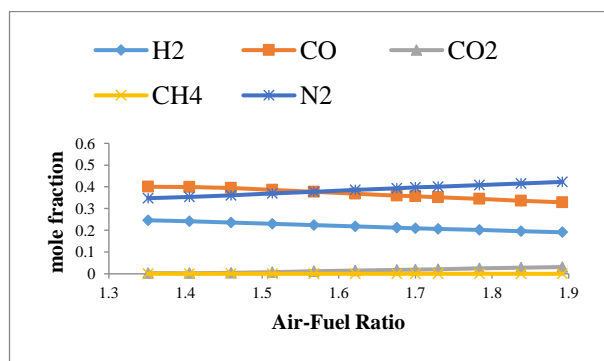


Fig. 5. Variation of syngas composition with air-fuel ratio

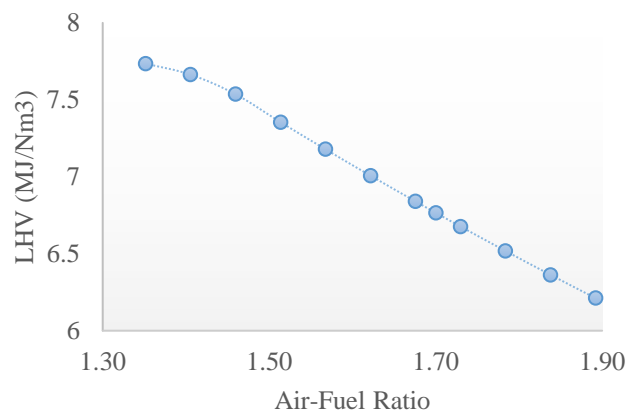


Fig. 6. Variation of LHV with air-fuel ratio

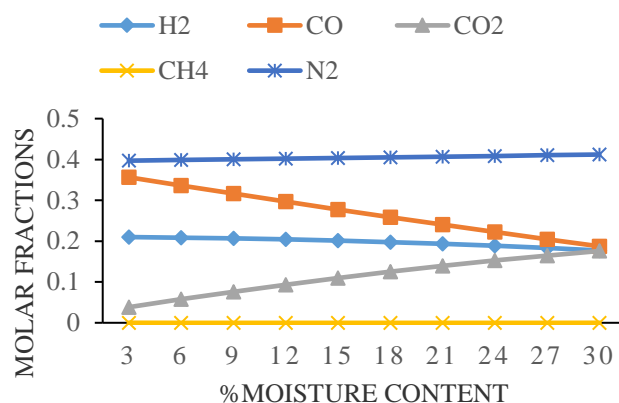
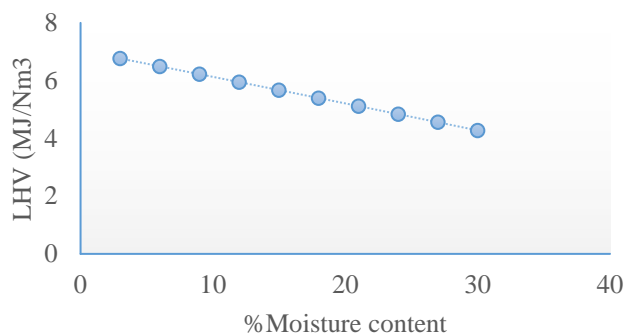


Fig. 7. Variation of syngas composition with moisture content

### 2.3.3. Effect of moisture content

The wood waste moisture content was varied from 3 to 30% to study its influence on syngas quality. Fig. 7 shows how the wood waste moisture levels affected the syngas composition. The analysis revealed that the mole fractions of CO and H<sub>2</sub> decreased while that of CO<sub>2</sub> increased and the mole fraction of N<sub>2</sub> increased slightly with increase in moisture content. Mole fraction of CH<sub>4</sub> although remains approximately constant, were quite insignificant with increase in moisture content. Similar trend were reported by [8, 13]. These variations is due to the fact that during gasification, moisture content favours production of more CO<sub>2</sub> according to water-gas shift reaction (Eq. 6). This is because higher moisture content results in low gasifier temperatures, as more heat is required to remove water from the feedstock. Hence, reduction in the energy content of produced syngas, because the little increase in H<sub>2</sub> is insufficient to make up for the significant loses of CO at high moisture levels [50, 51]. With air as the gasifying agent, the methane content is small and stays virtually constant with increase in moisture levels [12]. Fig. 8 presents variation of syngas lower heating value with biomass moisture content.



**Fig. 8.** Effects of moisture levels on syngas LHV

#### 4. Conclusion

Going by the obtained results, it can be concluded that:

- Air-gasification of wood wastes in a downdraft biomass gasifier was successfully modelled based on minimisation of Gibbs free energy using Aspen Plus.
- Predicted syngas composition was in fair agreement with measured syngas composition.
- Sensitivity analysis revealed that gasification temperature, air-fuel ratio, and biomass moisture level had significant effects on syngas quality.
- From the Aspen Plus model sensitivity analysis, it is recommended that to obtain syngas of good quality from the downdraft gasifier system, temperature should be between 750 – 950°C, air-fuel ratio should be between 1.35 – 1.51 and the biomass moisture level should not exceed 10%.

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