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Development of Model Systems Using Aspen Plus for Syngas Production from Waste via Gasification

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Abstract: The need for Energy is paramount to human existence. Biomass Gasification utilizes the process of synthesis gas "Syngas" production which can be used as an alternate to conventional means of energy generation. This Research encompasses the development of model systems using ASPEN Plus for syngas production from waste via gasification. The feed stock proximate and ultimate analysis used was obtained from previous authors whose research was done within Minna, Niger state. These obtained data were used to develop a model system using ASPEN PLUS simulation software and the Syngas composition H_2 , N_2 , CO, CO_2 , CH_4 . From table 5, model 3 and 4 of the Syngas composition were compared with the effective Syngas range of values, H_2 - 2-5%, CO- 35-40%, H_2 - 20-40%, CO_2 - 25-35%, CH_4 - 0-15%, which was within the range for effective Syngas. The obtained simulated Results show that the waste generated from these locations can generate an effective amount of Syngas that can be used for Energy Generation.

Keywords: Biomass Gasification, ASPEN PLUS, Model validation, SYNGAS, Energy Generation

1. INTRODUCTION

In Minna, Niger state where this research is based on, waste accumulation has steadily been on record high in Nigeria for as long as one can remember. The amount of waste generated increases with increase in economic growth in both developing and industrialized countries. Waste generation by the populace is highly significant, this is because of lack of proper disposal systems that should be put in place so as to minimize the pollution of the environment. One of this measures that should be in place is the "waste to energy" process plant which converts such waste into a source of clean energy, this waste could range from; domestic waste, farm waste, non-biodegradable waste etc. This proposed plant will reduce the dumping and litter of waste within the metropolis of Minna, air pollution, water pollution, dependency rate on fossil fuel generated energy and improve rate of recycling. Conversion of waste to high grade energy should not be the first solution of waste minimization, other strategies should be considered and exhausted, these could be prevention, reuse, recycling and minimization strategies. Thermal treatments are good options for waste reduction but it poses an adverse effect to the atmosphere. Effective and sustainable solutions to waste accumulation is a challenge to most developing countries, these solutions if applicable will not only solve the problem of pollution but also Global warming. A major part of this solution will be in the development of dependable sources of renewable energy and greatly reduce the dependency of conventional means of obtaining resources from reserves.

The suitable form of electricity used by residential buildings is of great importance to the energy sector, based on its end use compared to other methods or forms of energy generation. The use of wastes for electricity generation is not new, it has already been established and mostly used by developed countries like U.S.A, Sweden, India, Japan etc. In Nigeria, about 14 million tons of combustible solid waste are being produced on a yearly basis, out of which about 550,000 tons are generated in Niger state annually [1]. This establishes an environmental concern which are harmful and toxic to living things as well as it being disadvantageous to the surrounding and lifestyle. The transformation of such accumulated wastes or its mixtures is an important solution to these problems of pollution, sustainable energy generated from waste materials. Though, different methods are being used for these conversions, thermochemical processes are often seen to provide an encouraging double-usefulness for this problem: they greatly affect the amount of deposits present, while showing the merits of their calorific content and releasing a low toxic substance that can be used for energy generation [2]. In under developed countries, the knowledge on modern gasification processes is limited which leads to the waste being largely disposed of in dumpsites or incineration chambers.

The use of Syngas for energy generation in the form of electrical energy is of paramount importance to any country. In Nigeria where energy generation is not up to the minimum requirement. Hydroelectric, solar, wind, geothermal are known renewable energy sources, alternative methods should be employed, hence the use of gasification models. Gasification mostly involves the heating of waste residues to a high temperature, which breakdown particles into their elements in an oxygen limited atmosphere, which leads to the production of a final gas composed of hydrogen, carbon compounds and hydrocarbons that are short branched which may be used for energy generation, chemicals and liquid fuels [2]. Gasification can simply be defined as a thermochemical process that generates or converts organic or fossil based carbonaceous matters to carbon monoxide, Hydrogen, Carbon dioxide a gaseous, fuel rich product [3]. Gasification process involves the heating of the fuel (solid waste) with little oxygen to produce "syngas" which can be used to generate energy or as a source for methane, chemicals, biofuels or hydrogen production. The energy gotten from this process is higher compared to other thermochemical processes like combustion and pyrolysis. Gasification technology can majorly be used depending on the type of wastes, wastes are of two types: wet and dry wastes. Even though Gasification process technology has been in existence for almost two centuries, there has been a steady decline in its application due to cheaper and readily available petroleum and natural gas [4].

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Wet wastes which may include bio solids, food waste, manures are generally treated using biological processes while the Dry wastes (non-biodegradable plastics, crop stubbles, wood biomass etc.) are treated using thermal conversion processes such as combustion, gasification and pyrolysis.

Due to the extensive range of available waste, it is imperative to choose the most appropriate and fully compatible technology process that can give a high yield of the required product.

Other Solid waste technologies available for "waste to energy" are either based on biochemical conversions or thermal conversions [5].

The aim of this study was to develop models for the production of an effective Syngas using ASPEN PLUS. Conventional means of energy generation is usually not cost effective unlike the use of waste materials for Synthesis gas production which is clean energy.

2.0 GASIFICATION

The process of gasification has evolved over the years, but still retaining and improving on its importance. Gasification is commonly thought as unfinished burning/combustion. It is the combustion of solid fuels in the presence of minor amount of air (oxygen) giving an output gas that still retains its combustion potentials.

The processing of materials for gasification has been in existence for more than 180 years of which coal and peat were the primary fuel used to power gasification plants, these were used in the production of town gas for lighting and the production of fuels from wood to power motor vehicles [6].

Thermochemical process that effectuates a vaporous, fuel rich product can be termed gasification [3]. Gasification is a technology that use fuel to generate power and heat. This technology is also suitable for waste (farm waste, domestic waste, non-biodegradable waste etc.) conversion.

The exposure of filtrates to high temperature, which results to the breakdown of molecules into their elemental state in an environment of little oxygen or oxygen-deprived atmosphere, emitting an end-gas composed of H₂, CO, CO₂ and short-branched hydrocarbon which is usually used for energy generation, chemicals, hydrogen and liquid fuels is termed Gasification [13].

Gasification involves the oxidation of matter using a low amount of oxidizing agent below that of the stoichiometric need. The process is considered reliable, effective and an environmentally friendly way of generating energy [8].

2.1 Gasification process

The gas obtained through this process has been referred by different names by different publishers, some of the names are: producer gas, wood gas, generator gas, town gas, and commonly by synthetic gas or syngas.

In the process of true gasification five processes are usually involved, these processes are referred to as thermal processes: gasification/pyrolysis, combustion, cracking, reduction and drying, these processes are as you would expect present in any flame.

Pyrolysis involves an endothermic thermochemical process which requires carbonaceous disintegration of materials in the absence of oxygen. Pyrolysis is sometimes referred to as the first stage/process of thermal conversion. Due to the reduced temperature and lowering conditions, the pyrolysis of solid waste has the merits of lowering and reducing corrosion and emissions by keeping alkali, heavy metals, chlorine and sulphur in the process residue by reducing nitrogen formation, prevention of dioxins activation. Any process involving the breakdown of large complex particles such as domestic wastes, tars, solid agricultural wastes into less heavy or lighter gases in the presence of heat is termed Cracking. In thermal cracking the feed is heated and the molecules are disintegrated giving off a lighter gas, char and steam. Reduction is a process of peeling off oxygen atoms off burning products that are hydrocarbon in nature so as to turn these molecules to forms that are still combustible, ash and some char are usually the by-product of this reaction step. Reduction and combustion are opposite in process. Combustion involves the mixing of combustible gases with oxygen which produces water vapour and carbon dioxide waste product while reduction entails the removal of oxygen from these combustible gases. Reduction and combustion are equal and reverse reactions. Experiments carried out shows that they

both operate simultaneously in any burning environment in the form of dynamic balance moving back and forth between the two processes. Drying is a mass transfer process whereby moisture is evaporated from a material by the application of heat. The process of moisture removal in the biomass before entering the pyrolysis stage is termed drying. The moisture is usually removed from the feedstock before the process of gasification can begin. High moisture fuel availability and inadequate handling of the moisture content is one of the most re-occurring reasons for failure of gasification.

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2.2 Gasifiers

A gasifier is a largely used equipment in the process of gasification, it is characterized based on bed and flow (Energies, 2009). Gasifier bed is of two types fixed-bed gasifier and fluidized bed. Fixed bed gasifier can be further divided into updraft (counter current) or downdraft (concurrent). The conditioned parameters of a gasifier include but not limited to, type and design of gasifier, temperature of the gasification process, flow rate of the feed, oxidizing agents, type and amount of catalyst, feed nature and properties.

2.2.1 Synthesis gas "Syngas": Syngas is a fuel gas mixture these mixtures include: hydrogen, carbon monoxide, small quantities of carbon dioxide and minute trace gases. Syngas is usually generated or derived from feedstock; gasification of a carbon-based fuel leads to the production of syngas. Syngas constitutes 50% of the energy density of natural gas which makes it combustible and efficient as a fuel source [9].

In Syngas production, phases such as heating phase, reaction phase, purification phase and catalytic phase exists.

- 2.2.2 Power generation from Syngas: The major application of Syngas is in the power generation sector and heat. This can be obtained either in stand-alone combined heat and power plants or through co-firing of the syngas gas in large-scale power plants. Gasification syngas can be used for the production of power due to the fact that it is a combustible gas, different types of equipment from steam cycles through gas engines and turbines. For efficiency and effective production, consistent and stable fuel provided to the internal combustion engine is one of the main factors of the process.
- 2.2.3 Application of Syngas: Syngas is majorly used in the energy and power sector and can be used to produce different range of fertilizers, solvents and synthetic materials. Some applications of Syngas include:
- 1. Electricity generation using steam turbine drivers
- 2. Pressuring agents and fertilizer in the form of Nitrogen
- 3. Carbon-monoxide generation for use in chemical industrial feedstock and fuels
- 4. Hydrogen, for electricity generation: in refinery industries to extract more diesel and gasoline from crude oil in hydrogenation reactions
- 5. Elemental sulfur for chemical industries
- 6. Minerals and solids are mostly char, products of gasification, are used as roadbeds.
- 2.2.4 Simulation for gasification: The rapid cost-effective growth and technological enhancements of the last few decades together with the reckless depletion of the conventional method of power generation steadily increase the importance of the unconventional methods like Gasification which account for approximately 10% of the world production [10].

Commercially, the production of syngas from waste can be optimized by using certain simulation software which helps to show the feasibility of the feed stock and its theoretical production rate.

ASPEN PLUS, ASPEN HYSYS and CamCAD are the most commonly used simulation software used for biomass gasification, its graphical interface provides comprehensive integrated solutions to chemical Engineering problems involving designs [11]. For the purpose of this research the ASPEN PLUS simulation software would be used. This simulation software is convenient when solid and non-conventional feed stock are used. Different phases are encountered in ASPEN PLUS simulator they are, decomposition of the precursor biomass, volatile reactions, biomass gasification and gas separation [4].

Feed decomposition

Feed decomposition which usually involves non-conventional feed, the ASPEN PLUS yield reactor (MODEL ID: RYield) is used. It is commonly used when reaction stoichiometry is unidentified or unimportant. In this unit, the feed stock is transformed into its base component which include carbon, oxygen, hydrogen, sulphur, nitrogen and ash by the application of the ultimate and proximate analysis carried out.

Volatile reaction

The Gibbs reactor (MODEL ID: RGibbs) which is seen on the ASPEN simulation software <u>is</u> applicable for the model process. It is used when the reaction temperature coupled with the pressure are known and the stoichiometry reaction are not known. The gas phase partially consists of carbon which takes part in de-volatisation with the residual carbon found in the solid phase. The mixture is separated using a model separator to distinguish the ash from the gas mixture. Biomass gasification

For biomass and solid gasification, the RGibbs is also used to simulate gasification processes of the biomass. For char gasification, the Model CSTR performs the gasification process by applying reaction kinetics.

The simulated model obtained can be used as a predictive tool for optimization of the gasification process.

2.2.5 Relevance of simulation: ASPEN PLUS simulation software is of great importance in chemical Engineering design processes, the benefits include:

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- Reduced cost of production and purchase of engineering materials and equipment by designing and developing models so as to determine the relevant production path and the appropriate equipment to be used.
- Deduction of theoretical composition of the syngas which shows the degree of acceptance range for proper syngas production.
- Linear programming models and techniques among various mathematical optimization techniques have evolved through the years to optimize the gasification operations. Simulations are now used to help reduce the land mass and increase productivity of any gasification process, unnecessary units can easily be discarded and maximum products separation can be achieved using simulation.
- Process plant design path can be improved through the use of simulated software, for new designs, model designs can be quickly constructed depending on the process scenarios.

3.0 METHODOLOGY

The economic impact of utilization of waste is paramount in any country, the process of obtaining a suitable model design involves the collection of data (Proximate and ultimate analyses data) of wastes (Domestic, farm and municipal wastes) from previous authors and inputting into ASPEN PLUS simulation software. The characterization of waste materials can be done in relation to the Proximate and ultimate Analysis as well as in terms of energy value (heating value) as reported by previous researchers for various use excluding the application of gasification.

3.1 Equipment

For the course of this research, ASPEN PLUS v8.8 simulation software was used.

Other software that can be used include

- ChemkinPro software
- Comsol Multiphysics
- Ansys Fluent software
- ➤ Mathematica software
- ChemCAD
- MatLab
- Gasifier.exe
- ASPEN HYSYS

3.2 Precursor Biomass

The materials to be used for the process of gasification include but not limited to

- Farm waste; waste of cotton crops, rice husks, maize stalk, corn cobs, tree barks etc.
- Domestic waste; kitchen waste, household waste, litters
- Non-biodegradable waste; nylon, plastics

3.3 Methodology

To develop a model system for gasification, the following successive steps were used.

- 1. The specification of the stream class
- 2. The method employed for Property selection
- 3. System component specification and identification of conventional and non-conventional components
- 4. outlining the process flowsheet, using operation blocks for each unit and connecting materials and energy streams
- 5. Stipulating feed streams; flow rate, composition, and thermodynamic condition
- 6. Showing unit operation blocks (thermodynamic condition, chemical reactions, etc.) [1 and 2]

Assumptions made:

- 1. Operation on a Steady state platform, kinetic free conditions and isothermal processes
- 2. Chemical reactions should occur at an equilibrium state in the gasifier and there is no account of pressure loss
- 3. All elements participate in the chemical reaction
- 4. All gases used or produced are ideal gases as stipulated, including H₂, CO, CO₂, Steam (H₂O), N₂ and CH₄
- 5. Bottom product contains volatile matters made up usually of carbon, H_2 and O_2

6. Residues such as Tars and Char are assumed as non-equilibrium products, these reduces the hydrodynamic complexity.

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[1, 2, 4 and 10]

- 3.3.1 Model and process description: A number of processes are involved in gasification:
 - Drying
 - Pyrolysis/Decomposition
 - Reduction
 - Combustion
- 3.3.2 Model Development: A stoichiometric steady state model was developed to simulate non-conventional feed syngas gasification of wastes using ASPEN PLUS process software. An IDEAL property gas method was used. HCOALGEN and DCOALIGT were the enthalpy and density model selected for both feed and ash for non-conventional components The ASPEN PLUS flow sheet of the developed model was shown in fig. 1. Processes such as pyrolysis, reduction and combustion are integrated into the simulation by using FORTRAN statements. The proximate and ultimate data of waste was obtained from different authors; these data as denoted by unconventional feeds was used in ASPEN PLUS to develop a suitable model for Syngas production [1, 11 and 12].

Relevant equations in gasification:

FEED →O.O555H₂O C + O₂ → CO₂ C + 0.5O₂ → CO C + CO₂ → 2CO C + H₂O → CO + H₂ CO + H₂O → CO₂ + H₂ C + 2H₂ → CH₄ H₂ + 0.5O₂ → H₂O CH₄ + H₂O → CO + 3H₂ CH₄ + 2H₂O → CO₂ + 4H₂

Table 1: Operating Parameters

Table 1. Operating 1 arameters					
Model parameter	Feed	Air	Gasifier		
Flowrate, kg/h	100	1-100	-		
Pressure, bar	1	1	1		
Temperature, °C	25	25	500-1500		

Gasification of the waste materials starts with the drying process. The ASPEN PLUS stoichiometric reactor, RStoic with model ID DRIER was used to simulate the drying process. The drying process was controlled by writing a FORTRAN statement in the calculator block. The output from the DRIER was then separated using a separator model (ID: SEP1) with the evaporated moisture drained out of the process. The heat of reaction associated with the drier Q- DRIER was represented using an energy stream and then passed into the ASPEN PLUS yield reactor, RYield (model ID: DECOMP) where the feedstock was decomposed, at the yield reactor, feed is converted into its components which includes C, O₂, N₂, sulphur according to the yield distribution of the ultimate analysis. Gasification of the biomass was done using the ASPEN PLUS Gibbs reactor, RGibbs (ID: GASIFIER), the proximate analysis distribution was introduced to the gasifier with injected air stream. The gas produced was separated from the ash composition using a separator model SEP2 and then sent to the RGibbs reactor (ID: GASIF2). The syngas was separated from the final gasification product 'SEP3'. The description of the blocks used in ASPEN PLUS flow sheet was shown in table 2.

Table 2: ASPEN PLUS Blocks and Descriptions

Name in ASPEN PLUS	Model ID	Description
RStoic	DRIER	Simulate the evaporation of moisture from feed and converts a part
		of feed to form water
Sep	SEP1	Separator that extracts the moisture from the dry feed
RYield	DECOMP	Simulate the decomposition of the feed. It converts non-
		conventional feed into conventional components by using a
		FORTRAN statement
Mixer	MIX	Mixture of air and the decomposed components
RGibbs	GASIFIER	Simulate gasification of the biomass

PROCESS ROUTE OF "WASTE TO ENERGY" GASIFICATION

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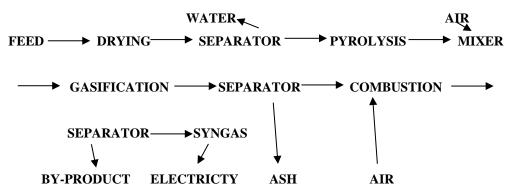


Table 1: Proximate Analysis of Waste from Different Authors [1, 11 and 12]

	PROXIMATE	ANALYSIS	DATA	
Feedstock	Moisture content %	Fixed carbon %	Volatile matter %	Ash %
Data 1				
Domestic waste (MSW)	19.32	23.17	44.40	12.11
Farm waste (corn stalk)	22.84	17.04	52.12	8.00
Data 2				
Rice husk	6.02	11.09	28.30	-
Wheat straw	2.82	18.76	78.41	-
Data 3				
Municipal solid waste	7.80	8.36	79.34	8.36
Data 4				
Solid domestic waste	7.01	16.08	75.90	1.09

Table 2: Ultimate Analysis of Various Waste [1, 11 and 12]

	ULTIMATE	ANALYSIS	DATA		
Feedstock	С	H_2	O_2	N_2	S
Data 1					
Domestic waste (MSW) %	65.56	5.91	27.27	1.26	-
Farm waste (sugar cane)	49.30	7.10	43.90	0.50	0.2
Data 2					
Rice husk %	39.82	5.63	48.07	0.8	-
Wheat straw	32.96	4.33	61.53	1.18	-
Data 3					
Municipal solid waste %	43.52	5.72	48.90	1.20	0.66
Data 4					
Solid domestic waste %	46.46	5.84	47.52	0.19	0.00

GENERAL MODEL DESIGN FOR WASTE GASIFICATION

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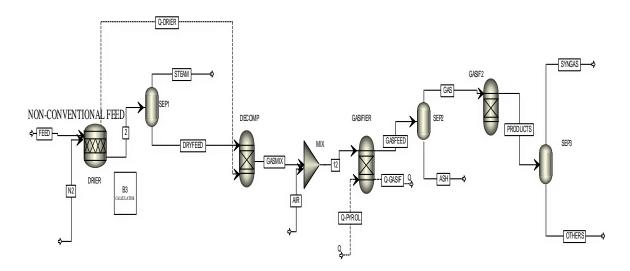


Figure 1: ASPEN PLUS simulation for waste to Syngas production

The data obtained was inputted into ASPEN Plus simulation software which shows the process in which the biomass can be used to produce Syngas for electrification. The simulated model was based on the Gibbs free energy minimization at equilibrium and also based under the assumption that the resident time was sufficient to allow the chemical reactions to reach an equilibrium state.

4.0 RESULTS

ASPEN PLUS results obtained from the proximate and ultimate analysis of data obtained from different authors.

FEEDSTOCK	\mathbf{H}_2	CO	CO ₂	CH ₄	N ₂	Others
MODEL 1						
Domestic waste	5.2	18.5	7.75	1.32	62.28	2.7
(MSW) %						
Farm waste (corn	4.89	12.09	11.38	3.2	65.72	2.72
stalk) %						
MODEL 2						
Rice husk %	27.71	22.92	35.51	12.43	0.90	0.60
Wheat straw %	15.67	29.77	41.09	3.09	10.39	-
MODEL 3						
Municipal solid	28.21	30.02	25.89	11.49	4.32	-
waste (MSW) %						
MODEL 4						
Solid domestic	44.89	38.21	21.20	11.39	4.87	1.53
waste %						

Table 3: Simulated Data of the Composition of Syngas using ASPEN PLUS

4.1 DISCUSSSION OF RESULTS

The application of ASPEN PLUS simulator for different feed stocks operating at different parameters of temperature, constant pressure, composition, constant mass input, different proximate and ultimate analysis obtained from previous researchers was studied and the simulated syngas composition obtained. It was observed that each model validation showed varying percent concentration. The residence time for the reaction is 1.2s on ASPEN PLUS.

For an effective Syngas, the syngas composition of most solid waste is;

- N2 2-5%
- ➤ CO 35-40%
- ➤ CO2 25-35%
- \rightarrow H2 20-40%
- ➤ CH4 0-15% [13]

4.4.1 Temperature: Temperature variations during Gasification process especially within the reactors has an effect on the composition of the produced gas (Syngas). Model validation for each Results shows that to obtain the Syngas, the gasifier (model I.D: RGibbs reactor) temperature should be above 1000°C. For any lesser temperature the yield of the by-product of the feedstock will be considerably small which in turn affects the concentration of the Syngas composition. To improve the concentration of the Syngas and effect proper separation, another RGibbs reactor is used operating with the same temperature. The hydrogen concentration which is one of the key components of the Syngas was 5.2% and 4.89%, with high nitrogen content 62.28% and 65.72% for Domestic waste and Farm waste under Model 1. The high nitrogen content can be attributed to the fact that the temperature used for this process was 800°C.

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From table 5, Model 2 shows the composition of the Syngas to be within the optimal conditions for an effective Syngas production with a slight deviation for the Wheat straw nitrogen content which was 10.39%.

Model 3 simulated result for the composition of the Syngas for Municipal Solid waste shows that the Theoretical Synthetic gas obtained will be an ideal and effective gas for energy generation. This proves that when the appropriate temperature variation conditions are met, the gas obtained will be an effective Syngas depending on the environment influence on the feed stock.

Model 4: The feed stock used was similar to the feed stock used in Result 3 (Solid domestic waste). Temperature variation as well as environmental influence constitute the composition of Syngas as show in table 13 (model validation).

4.4.2 Environmental Influence: The simulated results obtained from ASPEN PLUS can be attributed to environmental factors such as rainfall, soil content, high solar radiation and level of toxicity. These factors have great influence on the proximate and ultimate analysis as shown in the results obtained. The moisture content obtained from table 3 were within normal range except model 1 which was 48% and 29% for Domestic waste and corn stalk compared to other models whose moisture content ranged from 0-10%.

The location of the feed stocks analysed for the proximate and ultimate used for Syngas production were factors that greatly influenced the composition of Syngas that was simulated.

5. CONCLUSION

ASPEN PLUS simulation for gasification process is undeniably important for Syngas production. The compositions of syngas obtained can be related to an actual clean energy generation plant showing the possible output concentration and how feasible a feed stock is. The simulation using Gibbs Reactor which operates base on the reduction of Gibbs free energy and chemical and thermodynamic equilibrium shows how the composition of biomass obtained from different locations differ due to the difference in proximate and ultimate analysis. The obtained models were then compared to a standard+ model so as to determine the effectiveness of the syngas to be used for energy generation. Model results obtained from the simulation process as seen in table 5 shows the high hydrogen content of 28.21% and 44.89% for models 3 and 4 respectively, which is the determining component of Syngas for energy generation.

A stoichiometric steady state ASPEN model was obtained with minimum cost which was the objective of this research.

Gasification processes using simulations shows a clean and cost-effective means of waste treatment and can be used on a commercial scale for energy generation which helps to reduce pollution.

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