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Design of gasification process flow sheet with the chemical looping blocks in aspen plus

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Abstract

In order to improve hydrogen yield and carbon dioxide capture from Nigeria's abundant agro-waste, a downdraft gasification model was simulated using Aspen Plus, with blocks representing decomposition, oxidation, reduction, and syngas separation. The study looked at the effects of gasification parameters like steam-to-biomass ratio (SBR), equivalency ratio (ER), and steam-to-air ratio (SAR) on syngas yield, heating value, and cold gas efficiency (CGE). The results indicate that while increasing SBR improves hydrogen production, ER has a significant impact on syngas quality and carbon conversion. Using FeO_3 as an oxygen carrier, the integration of chemical looping modules showed enhanced CO_2 capture and increased hydrogen generation, making the system more ecologically friendly and sustainable. The results highlight how gasification and chemical looping can be combined to generate renewable energy and reduce carbon emissions in Nigeria.

Keywords: Gasification; Chemical Looping; Aspen Plus; Oxygen Carrier; Hydrogen production

1. Introduction

Nigeria, as one of Africa's largest agricultural producers, generates vast amounts of agro-waste annually. The country is a major producer of crops such as rice, sugarcane, palm oil, groundnuts, cocoa, etc. which are associated with significant agro-waste by-products (Akinbami *et al.,* 2011; Oladele and Oladipo, 2013). For instance, rice production in Nigeria results in large quantities of rice husks, which are often underutilized or discarded (Oloruntoba *et al*., 2018). Similarly, sugarcane bagasse, palm kernel shells, and groundnut shells are readily available in substantial quantities, especially in rural areas where these crops are processed (Onwuka *et al*., 2015). Nigeria is also one of the largest producers of cocoa in the world (FAO, 2024). It is ranked as the fourth-largest cocoa producer globally, after Côte d'Ivoire, Ghana, and Indonesia (FAO, 2024). Cocoa production is a significant part of Nigeria's agricultural economy, especially in the southern regions of the country, such as Ondo, Ekiti, and Akwa Ibom states. According to the Food and Agriculture Organization (FAO), Nigeria produces hundreds of thousands of metric tons of cocoa annually.

Research indicates that agro-waste in Nigeria has substantial energy potential. It is estimated that Nigeria produces over 20 million tons of agro-waste annually, much of which is underutilized (Akinbami *et al*., 2011). These residues, when properly harnessed, could significantly contribute to the country's energy needs, especially in rural areas where grid electricity supply is often unreliable or unavailable (Ogunwande *et al*., 2014).

Synthesis gas (syngas) is a key product of gasification and pyrolysis processes, produced by the partial oxidation or gasification of carbonaceous materials such as biomass, coal, and municipal solid waste. Syngas is primarily composed of carbon monoxide (CO), hydrogen (H_2), methane (CH_4), carbon dioxide (CO_2), and minor amounts of other gases like

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nitrogen (N_2) and sulfur compounds. The composition of syngas varies depending on the feedstock, the gasification process, and operational conditions (Li *et al*., 2020).

The syngas produced from gasification can be used in several applications such as:

- Power Generation: Syngas can fuel internal combustion engines, gas turbines, or fuel cells to generate electricity. Gasification-based power generation systems, particularly in combined heat and power (CHP) configurations, are becoming increasingly popular in decentralized energy systems (Patel *et al*., 2022).
- Biofuel Production: Through processes such as the Fischer-Tropsch synthesis, syngas can be further converted into liquid fuels like synthetic diesel, ethanol, and methanol (Li *et al.,* 2020). This is especially relevant as countries seek sustainable, carbon-neutral alternatives to fossil fuels.
- Industrial Chemicals: Syngas can serve as a feedstock for the production of a wide range of chemicals, including ammonia, methanol, and hydrogen, all of which are vital to industries such as agriculture, pharmaceuticals, and plastics production (Zhao *et al.,* 2021).

Several technologies are available for hydrogen production from agro-wastes, and their deployment in Nigeria could offer a sustainable pathway to energy security. Among these technologies, biomass gasification has emerged as a viable method for converting agro-wastes into hydrogen (Abdulkareem *et al*., 2020). Gasification involves the thermochemical conversion of biomass in an oxygen-controlled environment, producing syngas, from which hydrogen can be separated (Wang *et al*., 2018). Anaerobic digestion is another promising technology where organic material is broken down by microorganisms in the absence of oxygen, generating biogas, primarily methane, which can be reformed into hydrogen (Aremu *et al*., 2020).

The modeling and simulation approach plays a crucial role in the advancement of modern technologies, particularly in the field of chemical engineering and process development. Through the application of computer-aided process design tools such as Aspen Plus, engineers and researchers are able to model, simulate, and optimize complex industrial processes with a high degree of precision and efficiency (Zhang et al., 2019; Mustapha et al., 2024). This methodology supports a wide range of functions including plant design, operational analysis, process optimization, control strategies, and safety assessments. By providing a virtual platform for process experimentation, modeling and simulation significantly reduce the cost and risks associated with pilot-scale testing and real-life plant modifications (Enock et al., 2025).

Unlike traditional experimental methods, process modeling emphasizes the establishment of material and energy balances that describe the behavior of an entire system under varying operational conditions. This contrasts with flow field modeling and simulation, which primarily focuses on the spatial distribution and dispersion of physical quantities such as momentum, mass, and heat transfer within a given medium (Umetsu et al., 2014; Vekemans et al., 2023). While flow field simulation is more localized and often applied in fluid dynamics and thermal studies, process simulation aims to provide a holistic representation of interconnected unit operations within an industrial plant (Mustapha et al., 2024).

In practice, engineering solvers like Aspen Plus are employed to carry out these sophisticated calculations. The software utilizes thermodynamic models, kinetic parameters, and numerical algorithms to simulate steady-state and dynamic behaviors of chemical processes (Enock et al., 2025). This allows engineers to predict process performance, identify inefficiencies, and explore alternative design scenarios without physically constructing or modifying equipment. Moreover, the integration of optimization and sensitivity analysis tools within simulation environments facilitates decision-making by quantifying the impacts of design choices on energy consumption, cost, and environmental performance (Journal of Environmental Management, 2024).

Therefore, modeling and simulation not only serve as essential instruments for innovation in process industries but also act as enabling technologies that bridge theoretical knowledge with practical industrial applications. They enhance process reliability, safety, and sustainability by enabling systematic evaluation of operational strategies before implementation in real-life conditions (Mustapha et al., 2024; Vekemans et al., 2023).

2. Methodology

Using Aspen Plus software, the methodology for this study was organized around the modeling and simulation of a biomass gasification process combined with chemical looping modules. Model design, process unit specification, chemical reactions, assumptions, parameter adjustments, performance assessment, and chemical looping integration are among the steps required.

2.1. Process Modeling Framework

- Software Used: Aspen Plus v11 was employed as the primary modeling and simulation tool.
- Modeling Approach: A steady-state process model was developed to represent the thermochemical conversion of biomass into syngas in a downdraft gasifier.
- Feedstock: Agro-wastes such as cocoa pods were selected, and their proximate, ultimate, and sulfate analyses were inputted into Aspen Plus as the basis for simulation.

The process was represented by a sequence of Aspen Plus unit operation blocks as summarized in Table 1.

Table 1 Model blocks used in designing the downdraft gasification model

S/N	Unit	Function	Aspen Plus Block	Configuration
1	DECOMB	Biomass decomposition	RYIELD	Specified temperature = 500°C; Non-conventional component attribute = 100% Ash
2	COMB	Oxidation	RSTOIC	Operating temperature = 1000°C; Specified oxidation reactions
3	REACTOR	Reduction	RGIBBS	Calculation option = restricted chemical equilibrium; Operating pressure = 1 atm; Products = C (solid), other syngas components Specified reduction reactions
4	CYCLONE	Solid-gas separator	SSPLIT	Split fraction = 1
5	AIR-STM	Air-Steam Mixer	MIXER	
6	HX	Heat Exchanger	HEATX	Cold stream outlet temperature = 100°C
7	SEP	Liquid-gas separator	SEP	Outlet stream = SYNGAS Split fraction = 1

2.2. Chemical reaction modeling

The model incorporated key stages of biomass thermochemical conversion:

- Drying: Removal of moisture from biomass at 500 °C, producing dry feedstock and water vapor.
- Devolatilization: Decomposition of dry biomass into volatiles, char, and ash without oxygen.
- Volatile Reduction: Representation of volatiles by pseudo-compounds ($CH_aO_\beta N_d S_e$) decomposed into syngas components.
- Homogeneous Reactions: Included oxidation of CO, H_2, and C; partial oxidation of C.

2.3. Heterogeneous Reactions

- Boudouard reaction ($C + CO_2 \rightarrow 2CO$)
- Char reforming ($C + H_2O \rightarrow CO + H_2$)
- Water-gas shift ($CO + H_2O \rightarrow CO_2 + H_2$)
- Hydrogasification ($C + 2H_2 \rightarrow CH_4$)
- Steam/methane reforming ($CH_4 + H_2O \rightarrow CO + 3H_2$)
- H_2S and NH_3 formation reactions

2.4. Model Assumptions

2.4.1. General assumptions included

- Steady-state thermodynamic processes.
- Atmospheric pressure (1 atm).

- Char assumed to be pure carbon.
- Air composition taken as 79% N_2 and 21% O_2.
- Nitrogen considered inert.
- Peng-Robinson Equation of State applied.
- Oxidation and reduction zones treated separately due to temperature differences.
- Tar formation neglected.

2.4.2. Pyrolysis-specific assumptions:

- Temperature fixed at 500 °C.
- H_2O yield matched to biomass moisture content.
- All sulfur converted to H_2S; no NO_x formation.

2.4.3. Gasification-specific assumptions:

- No heat loss in DECOMP block.
- Carbon obtained as solid char/ash in reduction stage.

2.5. Gasification Parameters Investigated

Three key parameters were varied to assess process performance:

2.5.1. Steam-to-Biomass Ratio (SBR)

- Range: 0 – 2.0
- Objective: Enhance hydrogen yield through water-gas shift reactions.

2.5.2. Equivalence Ratio (ER)

- Range: 0.1 – 0.9
- Objective: Assess influence of air input on syngas yield and heating value.

2.5.3. Steam-to-Air Ratio (SAR)

- Range: 0 – 1.0
- Objective: Investigate syngas quality when both steam and air act as gasifying agents.

2.6. Performance Evaluation Metrics

To evaluate gasifier performance, three Key Performance Indicators (KPIs) were applied:

- Cold Gas Efficiency (CGE): Ratio of output syngas energy to input biomass energy.
- Lower Heating Value (LHV): Energy content of produced syngas based on constituent gases.
- Syngas Composition: Determined through Aspen Plus *Stream Results* (CO, H_2, CO_2, CH_4, N_2, etc.).

2.7. Chemical Looping Integration

- Objective: To enhance hydrogen yield and capture CO_2.
- Oxygen Carrier: Fe_2O_3 used as the looping medium.
- Blocks Added:
    - Reducer Unit: Converts Fe_2O_3 to FeO while oxidizing CO and H_2.
    - Oxidizer Unit: Re-oxidizes Fe and FeO with steam to produce H_2.
    - CO_2 Separation Unit: Captures and separates CO_2 from syngas.

2.7.1. Key Reactions in Reducer

- $Fe_2O_3 + CO \rightarrow 2FeO + CO_2$
- $Fe_2O_3 + H_2 \rightarrow 2FeO + H_2O$
- $FeO + CO \rightarrow Fe + CO_2$
- $FeO + H_2 \rightarrow Fe + H_2O$

2.7.2. Key Reactions in Oxidizer:

- $3Fe + 4H_2O \rightarrow Fe_3O_4 + 4H_2$
- $3FeO + H_2O \rightarrow Fe_3O_4 + H_2$

2.8. Simulation Flow

- Input feedstock composition (proximate and ultimate analyses).
- Define unit operations and reaction kinetics.
- Apply general and specific assumptions.
- Run base case simulation of downdraft gasifier.
- Vary SBR, ER, and SAR systematically.
- Record syngas composition, LHV, and CGE.
- Integrate chemical looping modules.
- Compare results with and without chemical looping.

3. Results

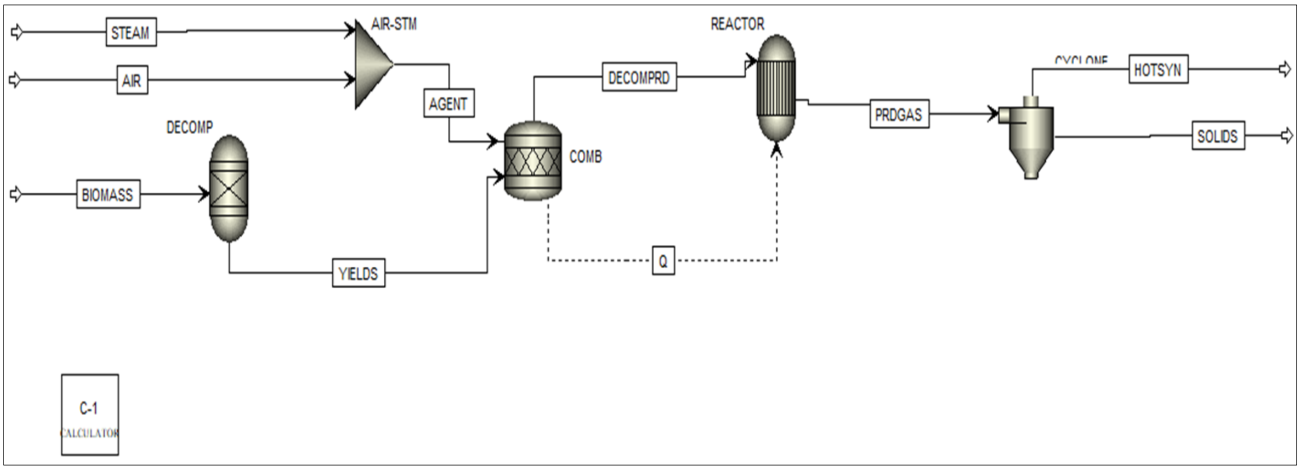


Figure 1 Downdraft gasifier model in Aspen Plus

3.1. Chemical Reaction Model

Chemical reactions in biomass gasification model involve the following processes: drying, devolatilization of biomass, homogenous reaction and heterogeneous reactions (Gupta et al., 2017b).

3.1.1. Drying

The drying model is given by Equation (1)

$$\text{Moist feedstock+ Heat} \rightarrow \text{Dry feedstock+ } H_2O_{(g)} \quad (2)$$

3.1.2. Devolatilization

The devolatilization model for biomass is given by Equation (3.). Decomposition of biomass is usually done in the absence of oxidizer

$$Dry\ Biomass\ \ \rightarrow Volatiles + Char + Ash + H_2O_{(g)} + inpurities\ (Tars, H_2S, dus \qquad (3.)$$

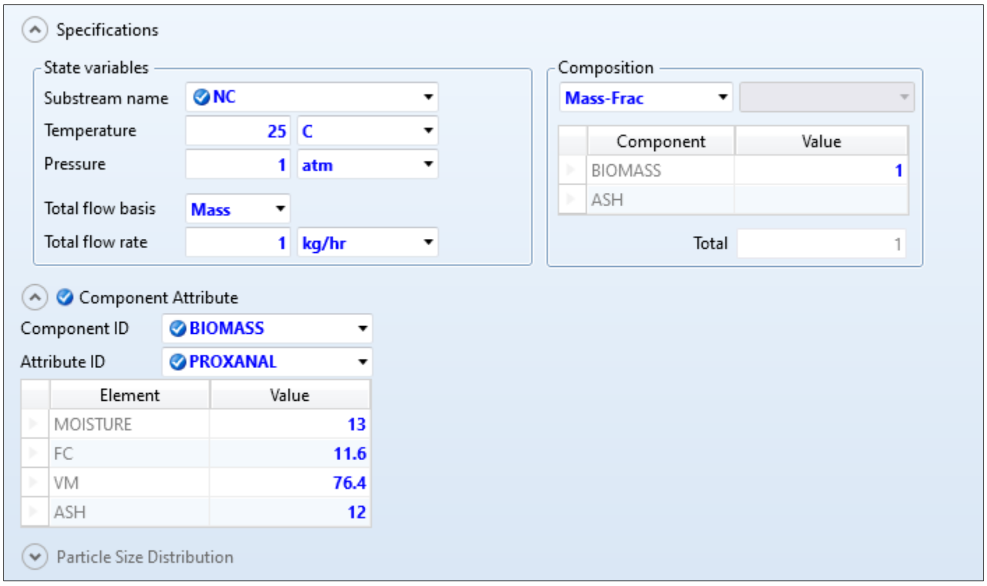
3.1.3. Volatile Reduction

A qualitative and quantitative knowledge of the devolatilization species is essential for realistic modelling of the coupled thermochemical conversion of food waste pellet into syngas (Janajreh and Al-Shrah, 2013; Jayathilake and Rudra, 2017).

Therefore, the volatiles, which are represented by a single molecule of the form $CH_aO_bN_d$are decomposed according to equation (4) which holds a strict balance of mass and heat into gas components (CO_2, H_2O, N_2).

$$CH_aO_bN_dS_e + v(O_2 + 3.76N_2) \rightarrow wCO_2 + xH_2O + yN_2 + zH_2S \qquad (4)$$

The chemical formula of biomass and volatiles are based on proximate and ultimate analyses of biomass chemical formula. Figures 2 to 4 depict the configuration of the proximate analysis, ultimate analysis and sulfate for cocoa pods respectively in the Aspen plus.



Specifications

State variables

Substream name: NC
Temperature: 25 C
Pressure: 1 atm
Total flow basis: Mass
Total flow rate: 1 kg/hr

Composition: Mass-Frac

Component	Value
BIOMASS	1
ASH	

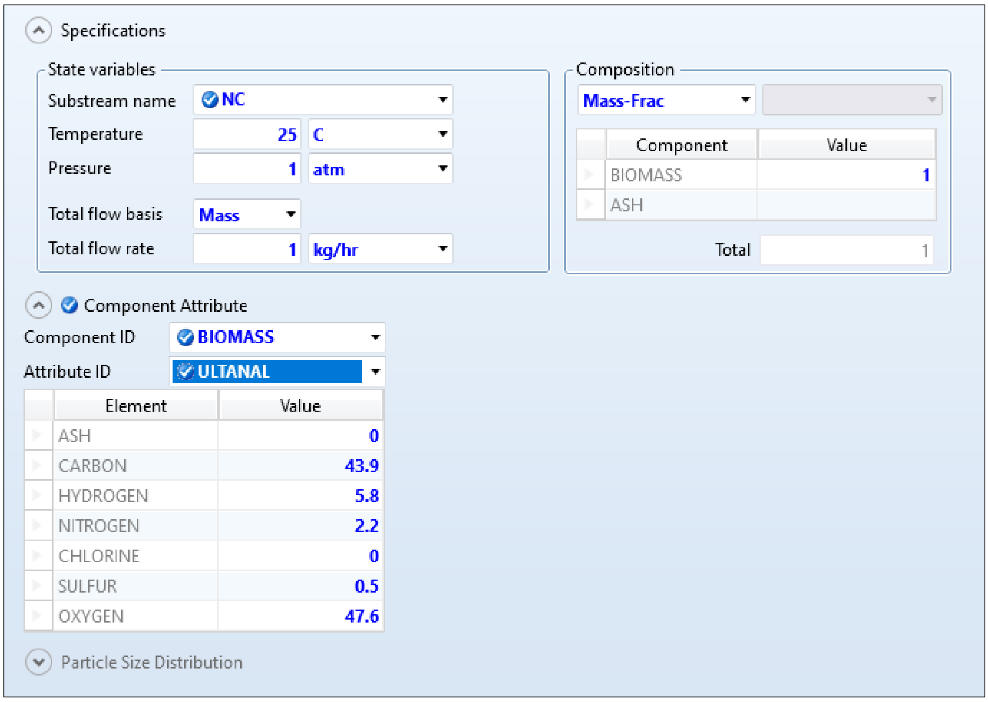
Total: 1

Component Attribute

Component ID: BIOMASS
Attribute ID: PROXANAL

Element	Value
MOISTURE	13
FC	11.6
VM	76.4
ASH	12

Figure 2 Configuration of the proximate analysis for cocoa pods in Aspen Plus



Specifications

State variables

Substream name: NC
Temperature: 25 C
Pressure: 1 atm
Total flow basis: Mass
Total flow rate: 1 kg/hr

Composition: Mass-Frac

Component	Value
BIOMASS	1
ASH	

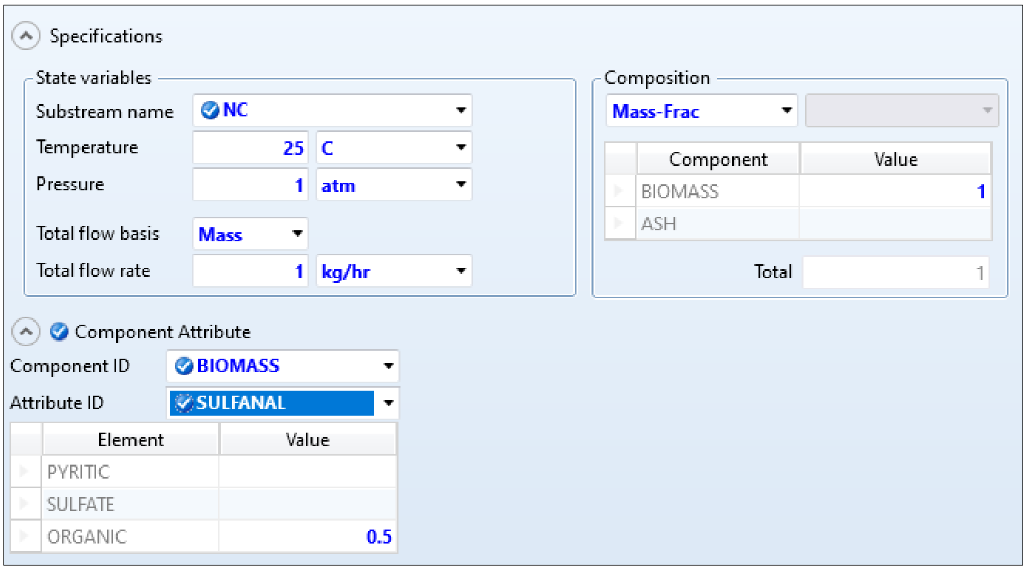
Total: 1

Component Attribute

Component ID: BIOMASS
Attribute ID: ULTANAL

Element	Value
ASH	0
CARBON	43.9
HYDROGEN	5.8
NITROGEN	2.2
CHLORINE	0
SULFUR	0.5
OXYGEN	47.6

Figure 3 Configuration of the ultimate analysis for cocoa pods in Aspen Plus



Specifications

State variables

Substream name: NC

Temperature: 25 C

Pressure: 1 atm

Total flow basis: Mass

Total flow rate: 1 kg/hr

Composition: Mass-Frac

Component	Value
BIOMASS	1
ASH	

Total: 1

Component Attribute

Component ID: BIOMASS

Attribute ID: SULFANAL

Element	Value
PYRITIC	
SULFATE	
ORGANIC	0.5

Figure 4 Configuration of the sulfate analysis for cocoa pods

3.2. Gas Phase Homogeneous Reactions

The various homogeneous reactions are given by Equations (5) to (7) (Slezak et al., 2010; Allesina et al., 2013), (Gupta et al., 2017b).

3.2.1. Oxidation of carbon monoxide

$$CO + 0.5O_2 \rightarrow CO_2 \qquad (5)$$

3.2.2. Oxidation of hydrogen

$$H_2 + 0.5O_2 \rightarrow H_2O \qquad (6)$$

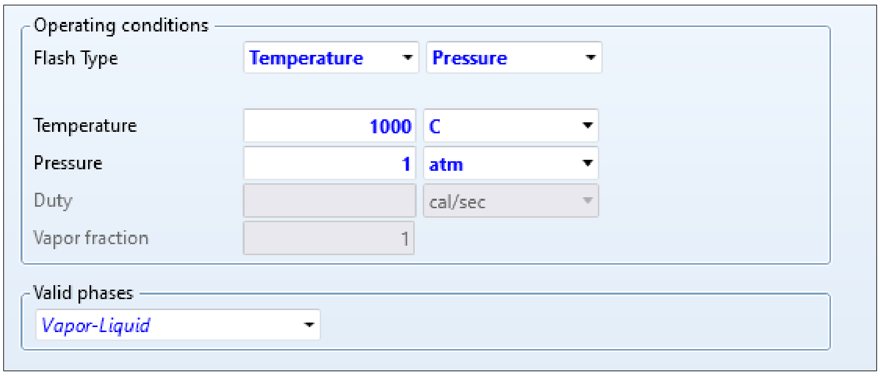
3.2.3. Oxidation of carbon

$$C + O2 \rightarrow CO2 \qquad (7)$$

3.2.4. Partial oxidation of carbon

$$C + 0.5\ O2 \rightarrow CO \ (8)$$

The operating conditions and the various reactions of the oxidation zone are shown in Figure 5 and 6 respectively.



Operating conditions

Flash Type: Temperature, Pressure

Temperature: 1000 C

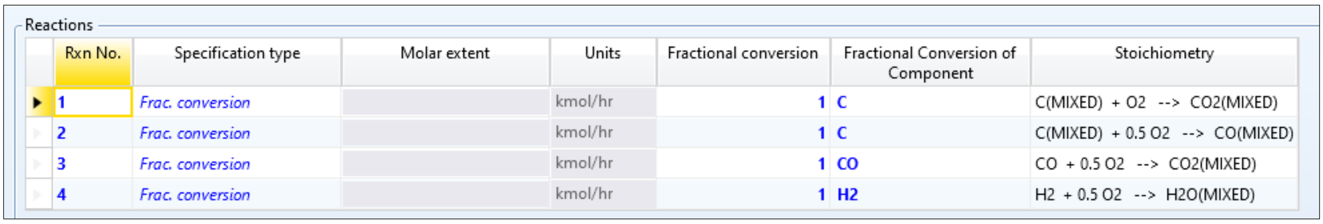
Pressure: 1 atm

Duty: cal/sec

Vapor fraction: 1

Valid phases: Vapor-Liquid

Figure 5 Oxidation zone configurations (COMB unit)



Reactions

Rxn No.	Specification type	Molar extent	Units	Fractional conversion	Fractional Conversion of Component	Stoichiometry
1	Frac. conversion		kmol/hr	1	C	C(MIXED) + O2 --> CO2(MIXED)
2	Frac. conversion		kmol/hr	1	C	C(MIXED) + 0.5 O2 --> CO(MIXED)
3	Frac. conversion		kmol/hr	1	CO	CO + 0.5 O2 --> CO2(MIXED)
4	Frac. conversion		kmol/hr	1	H2	H2 + 0.5 O2 --> H2O(MIXED)

Figure 6 Chemical equations for the oxidation zone

3.3. Particle Surface Heterogeneous Reaction

Multiple surface reaction models were used to model the food waste particles oxidation and gasification reactions. The heterogeneous equations are given by Equations (9) to (15) as seen in Arnavat, (2011); Gupta et al., (2017)

3.3.1. Boudouard reaction

$$C_{(s)} + CO_2 \rightarrow 2CO \qquad (9)$$

3.3.2. Char reforming reaction

$$C + H2O \rightarrow CO + H2(10)$$

3.3.3. Water gas shift reaction

$$CO + H2O \rightarrow CO2 + H2(11)$$

3.3.4. Hydrogasification reaction

$$C_{(s)} + 2H_2 \rightarrow CH_4 \qquad (12)$$

3.3.5. Steam/methane reforming reaction

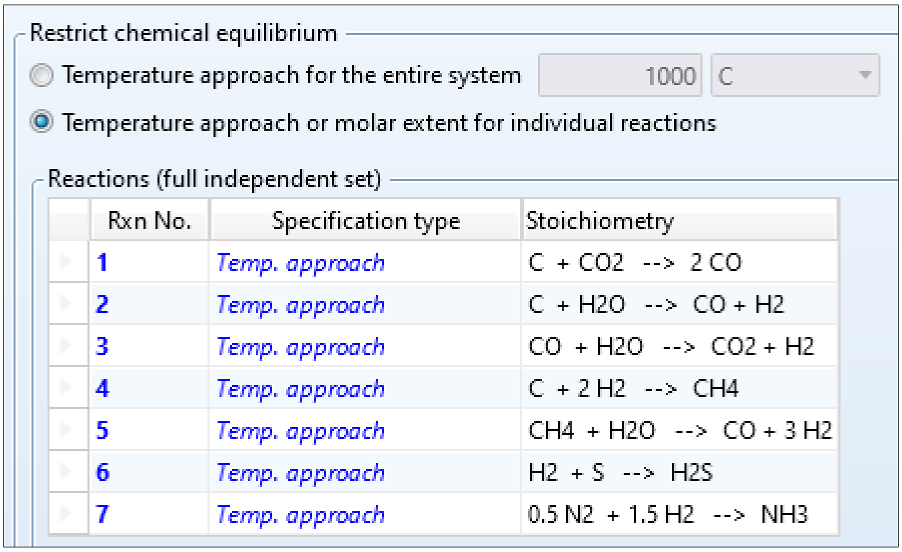
$$\mathrm{CH_4} + \mathrm{H_2O} \rightarrow CO + 3H_2 \qquad (13)$$

3.3.6. Hydrogen sulfide formation

$$H2 + S \rightarrow H2S \qquad (14)$$

3.3.7. Ammonia formation

$$0.5N2 + 1.5H2 \rightarrow NH3 \qquad (15)$$



Restrict chemical equilibrium

○ Temperature approach for the entire system 1000 C

● Temperature approach or molar extent for individual reactions

Reactions (full independent set)

Rxn No.	Specification type	Stoichiometry
1	Temp. approach	C + CO2 --> 2 CO
2	Temp. approach	C + H2O --> CO + H2
3	Temp. approach	CO + H2O --> CO2 + H2
4	Temp. approach	C + 2 H2 --> CH4
5	Temp. approach	CH4 + H2O --> CO + 3 H2
6	Temp. approach	H2 + S --> H2S
7	Temp. approach	0.5 N2 + 1.5 H2 --> NH3

Figure 7 Pyrolysis/reduction equations in Aspen Plus

Figure 7 shows the Aspen plus interface for inputting gasification Equation (9) to (15).

3.4. Model assumptions

3.4.1. General Assumptions

The general assumptions used for the model are

- All the thermodynamic processes are in a steady state.
- The pressure is atmospheric and remains constant.
- Char produced consists only of carbon.
- The composition of air is taken as 79% nitrogen and 21% oxygen on a molar basis.
- Nitrogen is an inert gas in the system.
- The Peng-Robinson equation of state was used for all the thermodynamic processes.
- Oxidation and reduction zones are separated in the model because their temperature differences are remarkably different, and
- The formation of tar has been neglected in this study.

3.4.2. Model assumptions for the pyrolysis process

The block's temperature was fixed at 500°C in accordance with conditions from the literature (Waheed et. al., 2024). Carbon, hydrogen, oxygen, nitrogen, and sulfur yields are to be computed based on the ultimate analysis of the biomass feed. The H_2O yield after pyrolysis was the same as the moisture content of the biomass feedstock. The entire sulfur in the feed is converted to H_2S, and no nitrogen oxides are produced. The heat that powers the pyrolysis process is derived from the heat of combustion.

3.4.3. Model assumptions for the gasification process

The main by-product of the process is char and tar, which are not formed at this stage. During oxidation, it is assumed that no heat loss occurred in the DECOMP block, while carbon is obtained as a pure solid in the form of char/ash as the by-product after reduction.

3.5. Gasification parameters

The three main gasification parameters that were considered in this study are firstly using air as gasifying agent thereby studying the equivalence ratio (ER), secondly using steam as gasifying agent thereby studying the steam to biomass ratio (STBR) and lastly using a combination of air and steam as gasifying agents thereby studying steam to air ratio (SAR). These were used to tune the gasifier oxidation agents' (air and steam) input flow rates. Output parameters investigated are the syngas composition, lower heating value (LHV) and cold gas efficiency (CGE) of the produced syngas.

3.5.1. Steam to Biomass Ratio

The steam-to-biomass ratio (SBR) is the ratio of the mass of steam injected into the gasifier to the mass of biomass input. The water shift reaction is enhanced with the increase in SBR, resulting in more production of H_2. SBR values between 0 and 2.0 was investigated in line with investigations of Tavares et al. (2020); Ahmad et. al., (2019); Anukam et. al., (2021); Basu Kaushal, (2020); Chen, Lin and Huang, (2022); Sun Chen and Yu, (2024); Vargas et. al., (2024). The steam flow rate was calculated with the expression of Equation. (16)

$$\text{Steam flow rate} = \text{SBR} \times \text{Biomass flow rate} \qquad (17)$$

3.5.2. Equivalence Ratio

The equivalence ratio (ER) is the ratio of the mass of air-to-fuel-ratio actual to the air-to-fuel-ratio stoichiometric amount required for oxidation. The conversion of the carbon in the biomass to syngas is enhanced with the increase in ER due to the availability of more oxygen. Paiva et al. (2021); Jayathilake and Rudra, (2017); Sarker and Nielsen, (2015); Zainal et al., (2001); Salisu, (2016) studied effect of equivalence ratio on syngas yield using wood, rice husk, millet husk as feedstock in a downdraft gasifier between the equivalent ratios of 0.1 and 0.9. However, for this study, equivalence ratio range of 0.1 and 0.9 will be investigated to determine the ER that will give the highest yield of syngas using the various fuel pellets. Equivalent ratio can be determined using Equation (18) as seen in Jayathilake and Rudra, (2017).

$$ER = \frac{Actual\ air\ fuel\ ratio}{Stoichiometric\ air\ fuel\ ratio} \qquad (18)$$

The actual air-fuel ratio can be determined from the measurement of the actual values of the masses of air and the fuel used for the experiment, while the stoichiometric air-fuel ratio can be determined from the ratio of mass of air to mass of fuel in the balanced gasification equation.

3.5.3. Steam to Air Ratio

Gasification experimental model was conducted using the downdraft gasifier in the Aspen Plus. The testing covered a range of Steam-to-Air Ratios from 0 to 1, based on literature recommendations (Hernández et al., 2012; Sharma and Sheth, 2016, Suyitno et. al., 2021; Salami, 2015). The steam flow rate was calculated with the expression of Equation. (19)

$$\text{Steam flow rate} = \text{SAR} \times \text{Air flow rate} \qquad (19)$$

3.6. Performance Analysis Metrics

Key performance indicators (KPIs) such as syngas composition, lower heating value and cold gas efficiency were used to evaluate the effectiveness of the gasification process.

3.6.1. Cold Gas Efficiency

Cold Gas Efficiency (CGE) is determined at each test condition as the output energy (heating value of the producer gas) divided by the input energy (heating value of the biomass) using Equation (20) as seen in Salisu, (2016).

$$CGE = \frac{LHV_{syngas} \times m_{syngas}}{m_{biomass} \times LHV_{biomass}} \times 100 \qquad (20)$$

Where:

- $LHV_{syngas} and\ LHV_{biomass}$ = Lower heating value of the syngas and biomass respectively,
- m_{syngas} = mass flow rate of the syngas in kg/s
- m_{syngas} = mass flow rate of the biomass in kg/s

3.6.2. Lower Heating Value

The lower heating value of the syngas is determined from the sum of the standard lower heating values of the combustible gases in the syngas produced. This is expresses mathematically by Equation (21).

$$LHV_{syngas} = \sum(LHV_i \times mm_i) \qquad (21)$$

$Where$:

$$mm_i = \text{mass fraction of specie i}$$

3.6.3. Syngas Composition

At the gasifier outlet (product stream), the mass flow rates of each syngas component (CO, H_2, CO_2, CH_4, N_2, H_2O, etc.) were extracted. The Stream Results function in Aspen Plus was used to access the detailed breakdown of all chemical species in the product stream. Molar fractions (%mol) and mass fractions (%wt) of the syngas constituents were recorded.

3.7. Chemical Looping

This section involves the simulation of the chemical looping of biomass-derived syngas using Fe_2O_3 as an oxygen carrier for efficient CO_2 capture and H_2 enhancement of the syngas using ASPEN Plus. The Chemical looping model involves the addition of the reducer and oxidizer blocks to the gasification model. Figure 8 show the Aspen Plus simulation model with the chemical looping modules.

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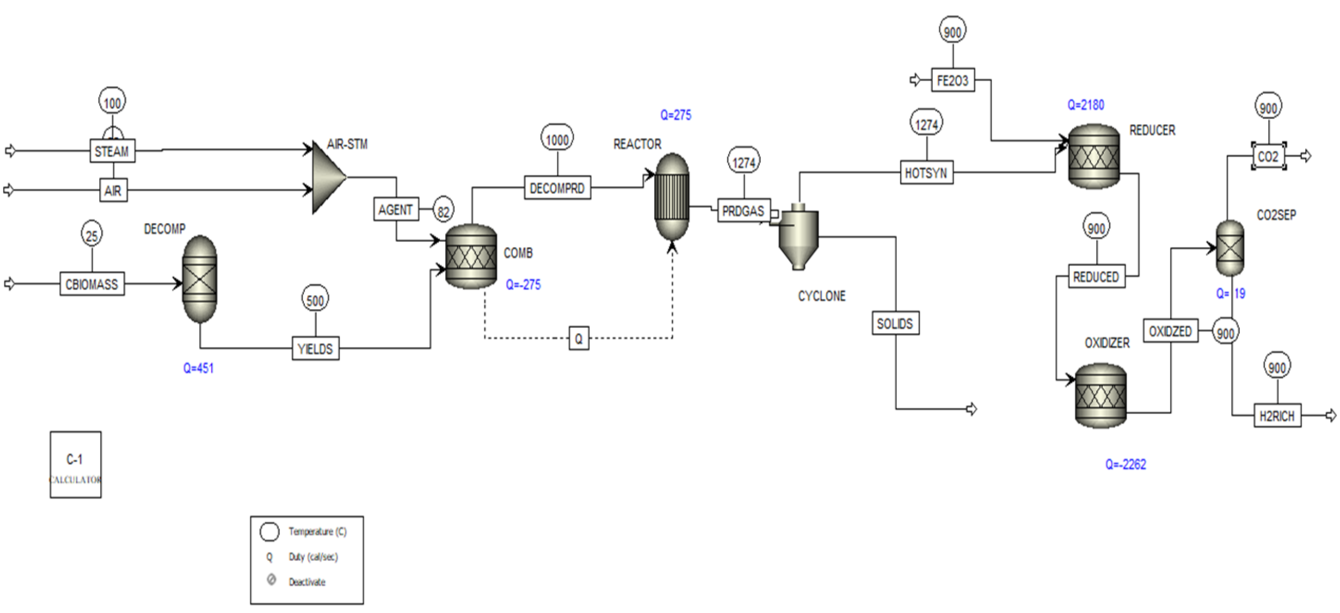
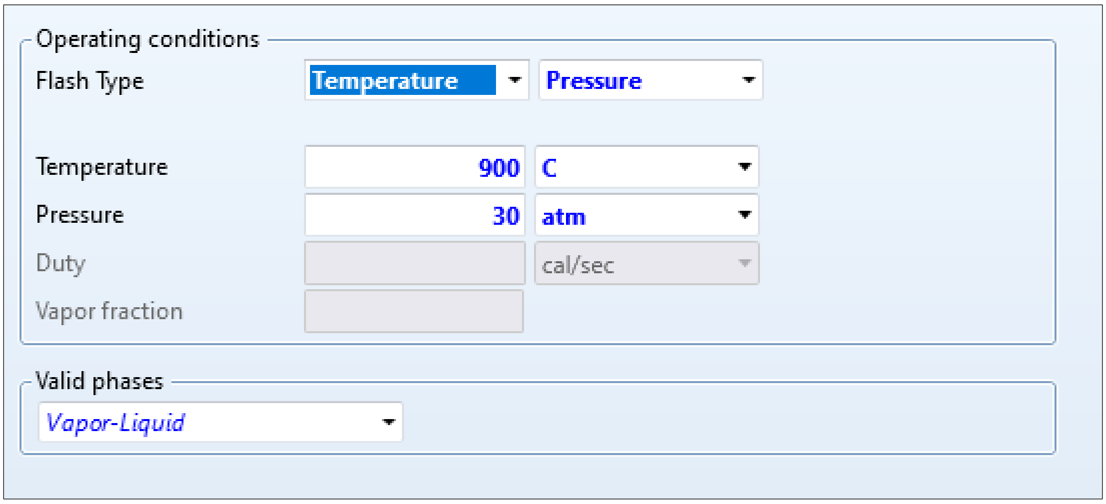


Figure 8 Gasification process flow sheet with the Chemical Looping Blocks

The operating conditions of the reducer and oxidizer units as inputted in Aspen plus are shown in Figure 9.



Operating conditions

Flash Type: Temperature, Pressure

Temperature: 900 C

Pressure: 30 atm

Duty: cal/sec

Vapor fraction:

Valid phases

Vapor-Liquid

Figure 9 Specifications for the reducer and oxidizer units

The model equations prevalent at the reducer units are presented in Equations 22 to 25.

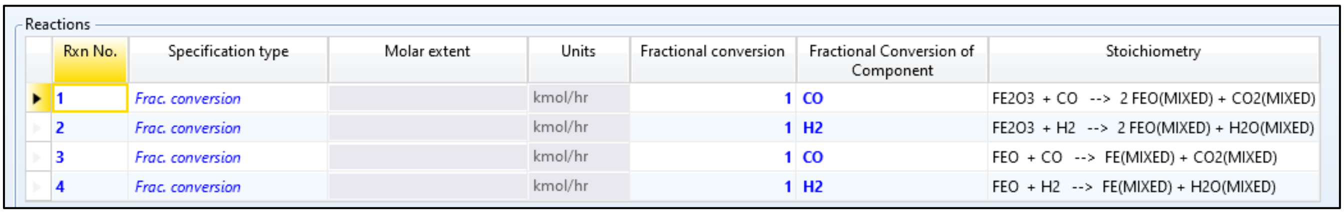
$$Fe_2O_3 + CO \rightarrow 2FeO + CO_2 \qquad (22)$$

$$Fe_2O_3 + H_2 \rightarrow 2FeO + H_2O \qquad (23)$$

$$FeO + CO \rightarrow Fe + CO_2 \qquad (24)$$

$$FeO + H_2 \rightarrow Fe + H_2O \qquad (25)$$

Figure 10 depict the Aspen plus configuration of the reducer model in the Aspen Plus.



Reactions

Rxn No.	Specification type	Molar extent	Units	Fractional conversion	Fractional Conversion of Component	Stoichiometry
1	Frac. conversion		kmol/hr	1	CO	FE2O3 + CO --> 2 FEO(MIXED) + CO2(MIXED)
2	Frac. conversion		kmol/hr	1	H2	FE2O3 + H2 --> 2 FEO(MIXED) + H2O(MIXED)
3	Frac. conversion		kmol/hr	1	CO	FEO + CO --> FE(MIXED) + CO2(MIXED)
4	Frac. conversion		kmol/hr	1	H2	FEO + H2 --> FE(MIXED) + H2O(MIXED)

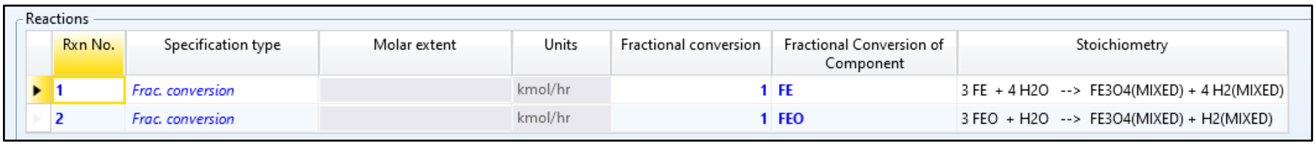
Figure 10 Reactions of the reducer in Aspen Plus

The model equations prevalent at the oxidizer units are presented in Equations 26 to 27.

$$3Fe + 4H_2O \rightarrow Fe_3O_4 + 4H_2 \qquad (26)$$

$$3FeO + H_2O \rightarrow Fe_3O_4 + H_2 \qquad (27)$$

Figure 11 depicts the Aspen plus configuration of the oxidizer models in the Aspen Plus.

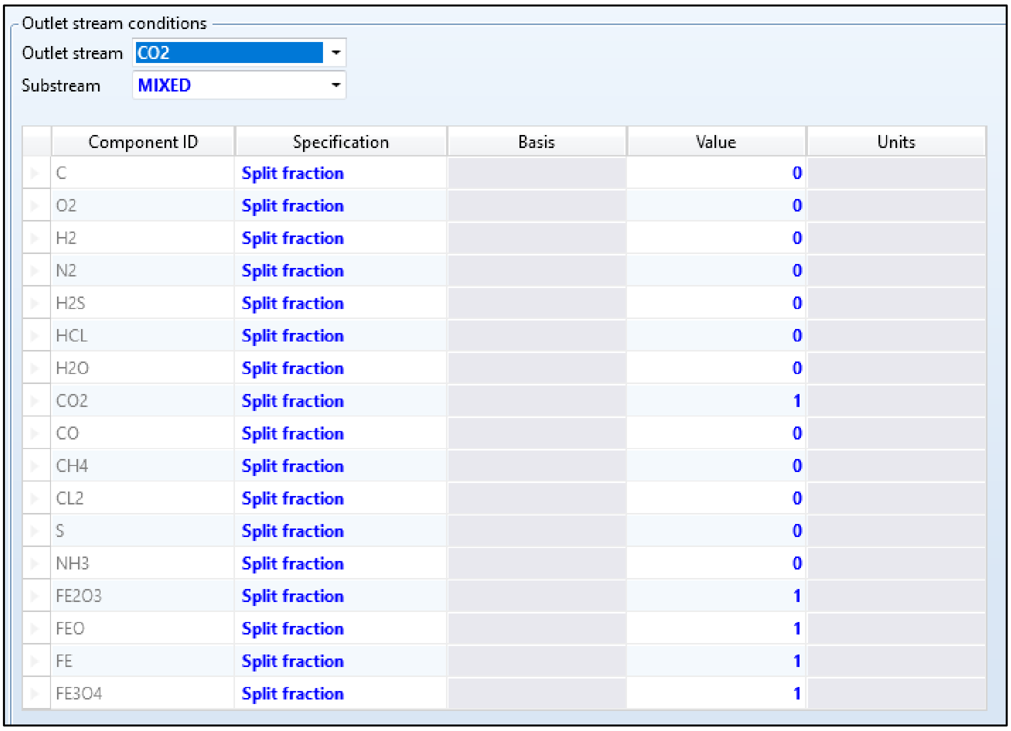


Reactions

Rxn No.	Specification type	Molar extent	Units	Fractional conversion	Fractional Conversion of Component	Stoichiometry
1	Frac. conversion		kmol/hr	1	FE	3 FE + 4 H2O --> FE3O4(MIXED) + 4 H2(MIXED)
2	Frac. conversion		kmol/hr	1	FEO	3 FEO + H2O --> FE3O4(MIXED) + H2(MIXED)

Figure 11 Reactions of the oxidizer in Aspen Plus

Figure 12 shows the CO_2 separation unit configuration in the Aspen plus model.



Outlet stream conditions

Outlet stream: CO2

Substream: MIXED

Component ID	Specification	Basis	Value	Units
C	Split fraction		0	
O2	Split fraction		0	
H2	Split fraction		0	
N2	Split fraction		0	
H2S	Split fraction		0	
HCL	Split fraction		0	
H2O	Split fraction		0	
CO2	Split fraction		1	
CO	Split fraction		0	
CH4	Split fraction		0	
CL2	Split fraction		0	
S	Split fraction		0	
NH3	Split fraction		0	
FE2O3	Split fraction		1	
FEO	Split fraction		1	
FE	Split fraction		1	
FE3O4	Split fraction		1	

Figure 12 CO_2 separation unit configuration in Aspen Plus

The chemical looping model was deployed at the exit of the gasification model in the Aspen plus for all the test conditions in order to enhance the hydrogen yield in the gasification modeling.

4. Discussion

The findings of the simulation demonstrate the technological feasibility of combining gasification with chemical looping to produce high-quality syngas from agricultural waste. The oxidation, reduction, and breakdown of biomass were well represented by the baseline Aspen Plus model, which produced syngas components such CO, H_2, CH_4, and CO_2. Higher steam-to-biomass ratios increased hydrogen yield through the water-gas shift reaction, as reported in previous research (Paiva et al., 2021; Vargas et al., 2024), and the impact of gasification parameters supported these findings. The balance between partial oxidation and complete combustion was also impacted by changes in the equivalency ratio, which in turn had an effect on the cold gas efficiency and syngas heating value.

By improving hydrogen concentration and making CO_2 capture easier, the incorporation of chemical looping offered substantial value. The selective oxidation of syngas ingredients made possible by reactions involving FeO_3/FeO cycles increased process efficiency. These findings are consistent with worldwide clean energy system trends that favor carbon capture, utilization, and storage (CCUS) technology more and more (Zhao et al., 2021). This strategy offers two solutions in Nigeria: it addresses rural populations' energy insecurity while reducing environmental issues related to the disposal of agro-waste. The results further illustrate Aspen Plus's usefulness as a potent process simulation tool that can connect theoretical concepts in chemical engineering with real-world advancements in renewable energy.

5. Conclusion

In order to produce hydrogen-rich syngas from Nigerian agro-wastes, this study constructed and simulated a gasification process flow sheet connected with chemical looping blocks. The findings showed that gasification parameters including the ratio of steam to biomass, equivalency, and air have a significant impact on syngas quality and process efficiency. Environmental performance was improved by the addition of chemical looping using FeO_3, which greatly increased hydrogen generation and made CO_2 capture possible. All things considered, the integrated process has a lot of promise for waste management, greenhouse gas reduction, and sustainable energy production in Nigeria.

Contribution to Knowledge

- Developed a comprehensive Aspen Plus model for downdraft biomass gasification incorporating decomposition, oxidation, reduction, and syngas separation blocks.
- Provided quantitative insights into how gasification parameters (SBR, ER, SAR) influence syngas composition, heating value, and efficiency.
- Demonstrated the technical feasibility of integrating chemical looping with biomass gasification for simultaneous hydrogen enhancement and CO_2 capture.
- Offered a replicable framework for using agricultural residues in Nigeria as feedstock for renewable energy, supporting national energy security and environmental goals.
- Bridged theoretical gasification and looping concepts with practical simulation techniques, strengthening process optimization for industrial application.

Recommendations

From the research carried-out it was recommended that;

- Policy Integration: Nigerian energy policies should promote the adoption of biomass gasification with chemical looping as a renewable energy strategy to reduce reliance on fossil fuels.
- Pilot-Scale Deployment: The simulation model should be scaled up into pilot projects using locally available agro-wastes such as cocoa pods and rice husks to validate the results in real-world conditions.
- Technology Investment: Government and private sectors should invest in process intensification and advanced separation technologies to enhance syngas purification and hydrogen recovery.
- Environmental Regulations: Adoption of chemical looping gasification should be encouraged as part of national CO_2 reduction commitments under climate change frameworks.
- Further Research: Future studies should explore multi-oxygen carrier systems, tar formation modeling, and life-cycle assessment (LCA) of the integrated process to assess long-term sustainability.

Compliance with ethical standards

Disclosure of conflict of interest

No conflict of interest to be disclosed.

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