Research Article

Optimization of Syngas Quality for Fischer-Tropsch Synthesis

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While fossil oil reserves have been receding, the demand for diesel and gasoline has been growing. In recent years, syngas of biomass origin has been emerging as a viable feedstock for Fischer-Tropsch (FT) synthesis, a process for manufacturing synthetic gasoline and diesel. This paper reports the optimization of syngas quality to match the FT synthesis requirement. The optimization model maximizes the thermal efficiency under the constraint of \( H_2/CO = 2.15 \) and operating conditions of equivalent ratio \( (ER = 0.0-1.0) \), steam to biomass ratio \( (SB = 0.0-5.0) \), and gasification temperature \( (T_g = 500°-1300°C) \). The optimization model is executed using the optimization section of the Model Analysis Tools of the Aspen Plus simulator. The model is tested using eleven (11) types of municipal solid waste (MSW). The optimum operating conditions under which the objective function and the constraint are satisfied are \( ER = 0 \), \( SB = 0.66-1.22 \), and \( T_g = 679-763°C \). Under optimal operating conditions, the syngas quality is \( H_2 = 52.38-58.67 \) mole percent, lower heating value \( (LHV) = 12.55-17.15 \) MJ/kg, and \( N_2 = 0.38-2.33 \) mole percent. From an economic point of view, 12.98% to 33.12% of biomass is used as fuel for steam generation, drying, and pyrolysis. The generalized optimization model reported could be extended to any other type of biomass and coal.

1. Introduction

High demand for transportation fuels stems from the growing world population, technological development, and surging transportation volume [1]. In recent years, the quest for feasible substitutes for fossil oil is intensified. Biomass is the most feasible alternative to fossil oil among renewable energy sources for many reasons. Biomass can provide alternative transportation fuels via Fischer-Tropsch (FT) synthesis, a process for the manufacture of synthetic gasoline [2–4]. The world production of biomass is estimated at 146 billion metric tons, equivalent to 14 Gtoe (based on an average higher heating value of 15 MJ/kg). This is more than three-fold the world’s primary energy demand of 14 Gtoe for the year 2020 [5]. Biomass constituents of C, N, and P can end up in waterways, increasing biochemical oxygen demand (BOD) and causing water pollution. The application of biomass for energy is a recommended solution for waste management [6]. In developing African countries, biomass is negatively priced; the price of biomass of agricultural origin is about USD 60 per ton on a dry basis, relative to the coal price of USD 400 per ton. Bearing in mind that coal’s heating value (25-35 MJ/kg) is about twofold that of biomass (10-20 MJ/kg). Biomass is CO₂ neutral; it absorbs CO₂ in the photosynthesis process to produce glucose as \[ C_6H_{12}O_6 + 6O_2 \rightarrow 6CO_2 + 6H_2O \]. In developing countries, biomass abundance and poverty coincide. Therefore, biomass utilization provides income and jobs and initiates socioeconomic development in poor nations. Biomass accounts for 35% of primary energy consumption in developing countries [7].

In light of the above, research on biomass gasification is a high priority. The challenge is to produce syngas with a quality that meets the FT synthesis requirement yet at a high gasification efficiency. This is the objective of this work. There has been a large volume of research on biomass gasification. Most of the existing research is on the influence of operating conditions and the type of biomass on syngas quality. The operating conditions are equivalence ratio \( (ER) \), steam to biomass ratio \( (SB) \), and gasification temperature \( (T_g) \). Recently, Rabah [8] studied the gasification of ten agricultural residues (bagasse, cotton stalks, sesame straw, groundnut shells, maize straw, sorghum straw, millet straw, sunflower husks, wheat straw, and banana leaves). Begum et al. [9] and Begum et al. [10] studied the gasification of...
coffee bean husks, green wastes, food wastes, MSW, pine sawdust, wood chip, and wood residue. Hlavsova et al. [11] studied nine composts obtained from nonhybrid and hybrid perennial grasses. Alex [12] studied prairie cordgrass and switchgrass. Rabah [13] investigated chicken manure. They established the range of the operating conditions as equivalent to 1 bar and considered isobaric and adiabatic. (4) The biomass is dried to 3% moisture at 1 bar and 150°C. (5) The dry biomass passes to the “RStoic” reactor (R-102) for pyrolysis. The “RYield” reactor block calculates the yield distribution of the products without the need to specify reaction stoichiometry and reaction kinetics [18]. The “RStoic” reactor converts biomass into conventional components (O₂, H₂, N₂, H₂O, S, tar, and char). The pyrolysis products (stream 5) are fed to the RGibbs reactor (R-103). The option of “Restrict chemical equilibrium-specify temperature approach or reactions” is chosen for the simulation of the RGibbs reactor. The reduction and oxidation reactions (Table 1) are supplied. The RGibbs reactor outlet (stream 6) moves to the cyclone (S-101), which separates stream 6 into wet syngas (stream 7) and ash (stream 8). The wet syngas (stream 7) is cooled in the heat exchanger (E-101), and the associated water is condensed. The cold wet syngas (stream 9) goes to the flash (V-102), which separates (stream 9) into syngas (stream 11) and water (stream 10). The air (stream 12) and steam (stream 13) as gasifying agents are added to the RGibbs reactor (R-103).

2.2. Process Simulation. Figure 1 shows the biomass gasification process flow diagram (PFD). The process description is attributed to Rabah [8] as below.

The wet biomass is fed into the “RStoic” reactor block (R-101), where moisture is liberated. The RStoic outlet stream (stream 2) goes into the separator (V-101), which separates the steam into moisture (stream 4) and dry biomass (stream 3). The dry biomass passes to the “RStoic” reactor (R-102) for pyrolysis. The “RYield” reactor block calculates the yield distribution of the products without the need to specify reaction stoichiometry and reaction kinetics [18]. The “RYield” reactor converts biomass into conventional components (O₂, H₂, N₂, H₂O, S, tar, and char). The pyrolysis products (stream 5) are fed to the RGibbs reactor (R-103). The option of “Restrict chemical equilibrium-specify temperature approach or reactions” is chosen for the simulation of the RGibbs reactor. The reduction and oxidation reactions (Table 1) are supplied. The RGibbs reactor outlet (stream 6) moves to the cyclone (S-101), which separates stream 6 into wet syngas (stream 7) and ash (stream 8).

2.3. Model Optimization. The optimization process is conducted using the optimization section of the Model Analysis Tool of the Aspen Plus simulator. Optimization requires the definition of the objective function, the constraint, and the variables under which the objective function and constraint are satisfied. The optimization process is modeled below:

\[ \eta = \frac{Q_o}{\sum Q_i}, \]

(1) Objective Function: the objective is the maximum thermal efficiency (\(\eta\)), which is defined by
where $\dot{Q}_o$ is the syngas energy content and $\sum \dot{Q}_i$ is the sum of energy input for biomass drying ($\dot{Q}_1$), pyrolysis ($\dot{Q}_2$), air heating ($\dot{Q}_3$), steam generation ($\dot{Q}_4$), and biomass energy content ($\dot{Q}_5$). $\sum \dot{Q}_i$ also includes energy recovery from hot syngas ($\dot{Q}_6$), moisture ($\dot{Q}_7$), ash ($\dot{Q}_8$), and loss to the surrounding ($\dot{Q}_9$).

(a) The energy output with the syngas is calculated as

$$\dot{Q}_o = \dot{M}_o \text{LHV},$$  \hspace{1cm} (2)

where $\dot{M}_o$ is the flow rate and LHV (MJ/kg) is the lower heating value of the syngas mass.

$$\text{LHV} = \sum y_i \text{LHV}_i, \ i = \text{H}_2, \text{CO}, \text{CH}_4,$$ \hspace{1cm} (3)

where $y$ is the weight fraction. LHV for $\text{H}_2$, $\text{CO}$, and $\text{CH}_4$ are 120, 10, and 50 MJ/kg, respectively.

(b) Drying: the energy input to the dryer is used to heat the solid biomass ($\dot{Q}_b$) and evaporate water ($\dot{Q}_w$). Under a diabasic drying condition, the energy balance is [19]

$$\dot{Q}_1 = \dot{Q}_b + \dot{Q}_w,$$

$$\dot{Q}_b = \dot{M}_b (C_{pb} + \omega i C_{pw}) (T_o - T_i),$$

$$\dot{Q}_w = \dot{M}_b (\omega i - \omega o) (\lambda + (C_{pw} - C_{pv}) T_o),$$

where $\dot{M}_b$ is the biomass flow rate, $C_{pb}$, $C_{pw}$, and $C_{pv}$ are the specific heats of biomass, water, and water vapor. The specific heat of biomass is 0.42 kJ/kg K. $T_i$ and $T_o$ are ambient and drying temperatures. To ensure efficient moisture removal, the drying temperature is taken as $T_o = 150^\circ \text{C}$. $\lambda$ is the water’s latent heat at 1 bar. $\omega_i$ and $\omega_o$ are the initial and final moisture content.

### Table 1: Biomass gasification chemical reactions [8].

<table>
<thead>
<tr>
<th>Phase</th>
<th>Reaction name</th>
<th>Biomass gasification</th>
<th>$\Delta H_r$ [kJ/mole]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Drying</td>
<td>Wet feedstock + heat = dryFeedstock + $H_2O$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pyrolysis</td>
<td></td>
<td>Dry feedstock+heat = char+volatiles</td>
<td></td>
</tr>
<tr>
<td>Oxidation</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Combustion</td>
<td>$C + O_2 = CO_2$</td>
<td>-394</td>
</tr>
<tr>
<td></td>
<td>Partial combustion</td>
<td>$C + 0.5O_2 = CO$</td>
<td>-111</td>
</tr>
<tr>
<td></td>
<td>Combustion</td>
<td>$H_2 + 0.5O_2 = H_2O$</td>
<td>-242</td>
</tr>
<tr>
<td>Reduction</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>C-water reaction</td>
<td>$C + H_2O \leftrightarrow CO + H_2$</td>
<td>131</td>
</tr>
<tr>
<td></td>
<td>Boudouard reaction</td>
<td>$C + CO_2 \leftrightarrow 2CO$</td>
<td>172</td>
</tr>
<tr>
<td></td>
<td>C-Methanation</td>
<td>$C + H_2 \leftrightarrow CH_4$</td>
<td>-75</td>
</tr>
<tr>
<td></td>
<td>Water gas shift</td>
<td>$CO + H_2O \leftrightarrow CO_2 + H_2$</td>
<td>-41</td>
</tr>
<tr>
<td></td>
<td>Steam reforming</td>
<td>$CH_4 + H_2O \leftrightarrow CO + 3H_2$</td>
<td>206</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$S + H_2 = H_2S$</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$Cl_2 + H_2 = 2HCL$</td>
<td></td>
</tr>
</tbody>
</table>

### Figure 1: PFD of biomass gasification.
(c) Pyrolysis: the total heat requirement for pyrolysis is the sum of the sensible heat for the temperature rise of biomass to the reaction temperature and the heat of the reaction as

\[
\dot{Q}_p = \Delta H_b + \Delta H_r^p,
\]

\[
\Delta H_b = \dot{M}_b C_{pb}(T_f - T_i),
\]

\[
\Delta H_r^p = \dot{M}_b(553 - 3142 x_{char}),
\]

where $x_{char}$ is the char concentration, $\dot{M}_b$ is the biomass flow rate, $C_{pb}$ is the biomass-specific heat ($C_{pb} = 0.42 \text{kJ/kgK}$), and $T_f$ and $T_i$ are the pyrolysis reactor and feed temperatures. The heat of the reaction is estimated based on the empirical equation (Equation (7)) of Antal [20].

(d) Air heating: the energy input for heating the air to gasification temperature is calculated using the first law of thermodynamics with zero work as

\[
\dot{Q}_a = \dot{M}_a C_{pa}(T_g - T_i),
\]

where $\dot{M}_a$ is the air mass flow rate, $T_i$ is the ambient temperature, $T_g$ is the gasification temperature, and $C_{pa}$ is the air-specific heat.

(e) Steam generation: the primary energy demand for steam generation is

\[
\dot{Q}_s = \dot{M}_s C_{ps}(T_g - T_i),
\]

where $\dot{M}_s$ is the steam flow rate, $C_{ps}$ is the steam-specific heat, and $T_g$ and $T_i$ are the steam generation temperatures, respectively. Steam generation is the major cost of biomass gasification.

(f) Biomass heating value: the biomass energy content is

\[
\dot{Q}_b = \dot{M}_b HHV.
\]

HHV of biomass is calculated using Dulong’s model given by

\[
HHV = 81|C| + 342.5\left(\frac{|H|}{8} + 22.5|S|,
\]

where HHV is in kcal/kg (1 kcal/kg = 4.187 kJ/kg), and $|C|$, $|H|$, $|O|$, and $|S|$ are the concentration of carbon, hydrogen, oxygen, and sulfur, respectively (see Table 2).

(g) Energy recovery from syngas: syngas leaves the gasifier at a higher temperature and needs to be cooled prior to the gas cleaning step (moisture removal). The cooling medium is water in a heat exchanger E101. Hence, the energy recovery from syngas is

\[
\dot{Q}_e = \dot{M}_g C_{pg}(T_g - T_o),
\]

where $\dot{M}_g$ is the syngas flow rate (including moisture), $C_{pg}$ is the syngas-specific heat, and $T_o$ is the syngas final temperature.

The energy input to pyrolysis is assumed to be integrated with energy recovery from the hot syngas in heat exchanger E101, energy escape with ash in cyclone S101, and moisture in the flash separator V101. This assumption is expected to make no significant error as steam generation and air heating are the major energy demands.

(2) Constraint: as noted earlier, the purpose of the present study is to optimize the operating conditions to produce syngas for FT synthesis. The principal chemical reactions for FT synthesis are:

\[
\text{Synthesis of paraffin: } (2n + 1)H_2 + nCO = C_nH_{(2n+2)} + nH_2O,
\]

\[
\text{Synthesis of olefins: } 2nH_2 + nCO = C_nH_{2n} + nH_2O.
\]

The reactions given by Equations (13) and (14) show that $H_2$ and CO need to be in a stoichiometric ratio of 2:1 or higher. Therefore, we choose to produce syngas with excess hydrogen; hence, the following ratio is considered.

\[
\frac{H_2}{CO} > 2.15.
\]

(3) Variables: the objective function and the constraint are functions of type of biomass, (HHV) and syngas quality (LHV, $H_2$, CO CH₄ concentration). As noted in the literature review, the operating conditions of ER, SB, and $T_g$ have a strong influence on syngas quality. These variables and their bounds are defined below.

ER is defined as the ratio of the actual and the stoichiometric air-fuel ratio (AFR) using the following

\[
\text{ER} = \frac{(\text{AFR})_a}{(\text{AFR})_s},
\]

where the subscripts $a$ and $s$ stand for actual and stoichiometric fuel-air ratio. AFR on a dry and ash-free basis (DAF) is calculated from ultimate analysis using the following:

\[
\text{AFR} = \left(\frac{|C|}{12} + \frac{|H|}{4} + \frac{|S|}{32} - \frac{|O|}{32} \right) \left(1 + \frac{79}{21} \right) \left(1 - \frac{\text{Ash}}{100} \right) \frac{28.4}{100}.
\]
The steam to biomass ratio (SB) is defined as

\[
SB = \frac{\text{Flow of H}_2\text{O as steam}[\text{kg/h}]}{\text{Flow of biomass}[\text{kg/h}]}. \tag{18}
\]

Stoichiometric steam to biomass ratio (SB) is

\[
SB = \left(\frac{C}{12}\right) \left(1 - \frac{\text{Ash}}{100}\right) \frac{18}{100}. \tag{19}
\]

(4) Variable bounds: the following bounds of the operating conditions are considered.

\[
\begin{align*}
0 & \leq \text{ER} \leq 1.0, \\
0 & \leq \text{SB} \leq 5.0, \\
500 & \leq T \leq 1300 + \text{C}.
\end{align*}
\]

2.4. Sensitivity Analysis. A parametric sensitivity analysis is performed to investigate the influence of the operating conditions (ER, SB, and \(T_g\)) on syngas quality. These operating conditions have the most influence on the gasification process. The sensitivity section of the Model Analysis Tools of the Aspen Plus simulator is run for the same range of ER, SB, and \(T_g\) considered in the optimization model. The performance is assessed with four measures, viz., syngas molar concentration of \(\text{CO}, \text{CO}_2, \text{H}_2,\) and \(\text{CH}_4;\) thermal efficiency; LHV; and \(\text{H}_2/\text{CO} \text{ molar ratio.}\)

3. Results and Discussions

3.1. Material Characteristics. Table 2 shows eleven MSWs, randomly selected from different sources. The selected MSWs have been used previously in simulation and experimental gasification research. The main characteristics of MSW are moisture, proximate and ultimate analyses, and HHV. The major components of MSW are organic, paper, plastic, metal, glass, and others (electric light, batteries, automotive parts, medicines, and chemicals). MSW characteristics depend on its composition and vary from community to community.

HHV is a function of carbon, hydrogen, and sulfur content as given by Equation (11). Carbon is the major component of biomass, followed by hydrogen and sulfur. Hydrogen has the highest calorific value of 120 MJ/kg, followed by carbon (33.74 MJ/kg) and sulfur (9.3 MJ/kg). The carbon content for MSW ranges from 31 to 58% by weight, while hydrogen and sulfur account for less than 8 and 1 percent by weight, respectively. Not all carbon is available for heat, because oxygen partially oxidized the carbon, decreasing its ability to generate heat. Similarly, not all hydrogen is available for heat because part of the hydrogen combines with oxygen to form water vapor according to the combustion reaction \((\text{H}_2 + 0.5\text{O}_2 = \text{H}_2\text{O})\). The hydrogen available for heat is thus \([(\text{H}) - (\text{O})]/8). Hence, the higher the carbon and hydrogen contents the higher the heating value, and the higher the oxygen content the lower the heating value.

MSW11 has HHV close to that of coal (25 to 35 MJ/kg) because of its higher carbon and hydrogen and lower oxygen content relative to other MSWs.

Table 2 shows AFR, and SB was calculated using Equations (16)–(19) on a DAF basis. The calculated AFR is based on the complete combustion of all biomass. In gasification, complete combustion is needed only to meet the energy demand for endothermic reduction reactions. Hence, ER should be minimum \((ER < 1)\) to avoid complete combustion. SB is calculated based on the C-water reaction \((\text{C} + \text{H}_2\text{O} = \text{CO} + \text{H}_2)).\) In gasification, besides the C-water reaction, steam is required for water gas shift \((\text{CO} + \text{H}_2\text{O} = \text{H}_2 + \text{CO}_2))\) and steam reforming \((\text{CH}_4 + \text{H}_2\text{O} = \text{CO} + 3\text{H}_2))\) reactions. Hence, the actual SB should be higher than the stoichiometric value shown in Table 2.

3.2. Model Validation. The results of the simulation model are compared with the simulation data of Suwatthiku et al. [30] at the same operating conditions (ER, SB, and \(T_g\)). The relative error is estimated as

![Table 2: MSW proximate and ultimate analyses, AFR, and SB on DAF basis.](image-url)
where $y$ is the mole fraction of syngas composition (H$_2$, CO, CO$_2$, and CH$_4$). The subscripts $a$ and $b$ stand for the present and Suwatthiku et al.’s [30] works, respectively. $i$ is the counter and $n$ is the total number of points. The mean square error (MSE) and the root mean square error (RMSE) are estimated using Equations (22) and (23).

$$\text{MSE} = \frac{1}{n} \sum_{i=1}^{n} E_i^2,$$

$$\text{RMSE} = \sqrt{\text{MSE}}.$$

Table 3 shows the proximate and ultimate analyses of the biomass used for comparison with Suwatthiku et al.’s [30] simulation.

Table 4 shows the operating conditions (ER, SB, and $T_g$), the present and Suwatthiku et al.’s [30] simulation results, and the statistical parameters. Besides (H$_2$, CO, CO$_2$, CH$_4$), syngas also contains H$_2$O and traces of N$_2$, H$_2$S, and HCl. However, for the sake of comparison, the syngas composition is normalized to (H$_2$, CO, CO$_2$, and CH$_4$). The present work predicts Suwatthiku et al.’s [30] results with a RMSE of 0.20, 0.23, 0.39, and 1.0 for H$_2$, CO, CO$_2$, and CH$_4$, respectively. It can be observed that the present results are in good agreement with Suwatthiku et al.’s [30] results for the case of H$_2$, CO, and CO$_2$ and in poor agreement with CH$_4$. The poor match for the case of CH$_4$ is attributed to the fact that the minimum formation of methane is a common problem experienced by many simulations works [8, 31].

3.3. Optimization Results. Table 5 shows the optimization results. It includes the following information:

(1) Optimal operating conditions (ER, SB, $T_g$) and efficiency

(2) Syngas characteristics: compositions (H$_2$, CO, CO$_2$, CH$_4$, N$_2$, H$_2$O, H$_2$S, and HCl) and thermophysical properties ($\rho$, MW, and LHV)

(3) Other variables: biomass flow rate ($\dot{M}_b$), syngas flow rate ($\dot{M}_s$), yield, and biomass used as a fuel ($\Delta$)

(i) Compositions are in mole % except CH$_4$, H$_2$S, and HCl are in ppm. (ii) All parameters have usual SI units. (iii) $Y = \text{Yield} = \frac{\dot{M}_s}{\dot{M}_b}$, where $\dot{M}_s$ and $\dot{M}_b$ are the syngas and biomass mass flow rates, respectively. (iv) $\eta$ and $\Delta$ are in %.

3.3.1. Optimal Operating Conditions

(1) Equivalent Ratio (ER). The optimization returned ER = 0, indicating no external air is needed. There are mainly three sources of oxygen for combustion reaction, viz., biomass, steam, and external air. The oxygen in the biomass is between 10% and 40% (see Table 2). Steam contains 89% oxygen and 11% hydrogen (oxygen contribution by water molecules). These two sources provide adequate oxygen for the partial combustion reaction. The advantages of ER = 0 are zero energy input for air and minimum nitrogen in the syngas.

(2) Steam to Biomass Ratio (SB). Table 5 shows SB for different types of MSW. The optimum SB is 0.66 ≤ SB ≤ 1.22. Chang et al. [32] and Molino et al. [33] reported the optimal SB value in the range of 0.3-1.0. The main sources of steam are steam input, moisture content, and steam generated in the combustion reaction (H$_2 + 0.5O_2 \leftrightarrow H_2O$). The steam is consumed in C-water, water gas shift, and steam reforming reactions. The advantage of steam gasification is the enhancement of H$_2$ and LHV in syngas. In practice, the energy input for steam generation is supplied by biomass as a fuel. Hence, it is important to estimate the percentage of biomass used as a fuel in steam generation. This is estimated as:

$$\Delta_t = \frac{\dot{Q}_t}{\eta_bQ_5} \times 100\%,$$

where $\Delta$ is the % of biomass used as fuel in steam generation, $\eta_b$ is the boiler efficiency, $Q_t$ is the energy input with steam (see Equation (9)), and $Q_5$ is the energy input with biomass (see Equation (10)). With a boiler efficiency of 80%, the biomass fuel for steam generation is $\Delta_t = 7.16$-22.69% of the total biomass.

Likewise, the biomass used as a fuel for drying is

$$\Delta_d = \frac{\dot{Q}_d}{\eta_bQ_5} \times 100\%,$$

and for pyrolysis is

$$\Delta_p = \frac{\dot{Q}_p}{\eta_bQ_5} \times 100\%.$$

With dryer and pyrolysis thermal efficiency of 80%, the biomass used a fuel for drying and pyrolysis are $\Delta_d = 0.38$-16.48% and $\Delta_p = 0.75$-4.11% of the total biomass, respectively. The total biomass used as fuel for steam generation, drying, and pyrolysis is in the range of 12.98%-33.12% (see Table 2).

(3) Gasification Temperature $T_g$. The optimal gasification temperature is $T_g = 679$-763°C. Pala et al. [3] reported $T_g = 800$-900°C. Buragohain et al. [2] reported the optimal conditions for the gasifier for FT synthesis purposes as $T_g = 800$-1000°C. The present work returned significantly lower $T_g$ than Buragohain et al.’s [2] model. However, it is noted that the previous research used air as the gasification medium, i.e., SB = 0. This justifies the high gasification temperature of the previous works. Lower $T_g$ tends to lower energy consumption, tar, and NOx formation.
(4) Efficiency. Table 5 shows the gasification efficiency estimated using Equation (1). The major energy consumption processes are drying, pyrolysis, and gasification. The minimum and maximum efficiency are 49% and 85% for MSW1 to MSW9. However, MSW10 and MSW11 experienced abnormally high efficiencies of 93% and 94%, respectively. This could be attributed to the low moisture content of MSW10 (8.03%) and MSW11 (3.30%); the moisture content of MSW1 to MSW9 is in the range of 12-52% (see Table 2).

3.3.2. Syngas Quality

(1) Syngas Composition. Syngas composition is shown in Table 5. The major syngas compositions are H₂, CO, and CO₂. The optimization returned zero concentrations of S and Cl₂, C, and O₂, and traces (in ppm) of CH₄, H₂S, and HCl. The hydrogen concentration varies between 52.38% and 58.67%. The hydrogen sources are hydrogen in the feedstock is 4.62-7.74% (Table 2), hydrogen that comes through steam (steam consists of 11% hydrogen and 89% oxygen), and hydrogen generated through C-water, water gas shift, and steam reforming reactions. The hydrogen is depleted by combustion reaction \( \text{H}_2 + \frac{1}{2}\text{O}_2 \rightarrow \text{H}_2\text{O} \), C-methylation reaction \( \text{C} + \text{H}_2 \rightarrow \text{CH}_4 \), and reaction with S \( \text{S} + \text{H}_2 \rightarrow \text{H}_2\text{S} \) and \( \text{Cl}_2 + \text{H}_2 \rightarrow 2\text{HCl} \). The high concentration of H₂ is thus may attribute to no occurrence of combustion and C-methylation reactions. The CO concentration may be attributed to the high conversion of the CO production reaction and the backward shift of the water gas reaction to reactants. The CO₂ concentration varies between 6.21 and 14.74%. The source of CO₂ is combustion and the water gas shift reaction. CO₂ is depleted by Boudouard’s reaction. Clearly, the low concentration of CO₂ may be attributed to high conversion by Boudouard’s reaction and the backward shift of the water gas shift reaction. Zero concentrations of S and Cl₂ is due to complete conversion into H₂S and HCl. Zero concentrations of C and O₂ are indicative to complete the conversion of C into CO and CO₂. The low concentration of CH₄ may be attributed to the high conversion of the steam reforming reaction.

3.4. Sensitivity Analysis. As indicated earlier, the performance of the gasification process has been assessed with two measures, viz., syngas molar concentration (CO, CO₂, H₂, and CH₄), efficiency, and H₂/CO molar ratio. The influence of \( T_g \), SB, and ER on these performance measures is presented. A sample of the results is discussed in the following subsections; the rest of the results (not shown here) show the same.

3.4.1. Influence of \( T_g \) on Syngas Quality. Figure 2 shows the influence of \( T_g \) on CO, CO₂, H₂, and CH₄ molar fraction in the range of 500°C-1300°C at constant ER and SB. As \( T_g \) increases, CO and CO₂ assume opposite trends and reach a point of crossover. The decrease in CO₂ could be attributed to the Boudouard reaction and the deficiency of O₂ for complete conversion into H₂S and HCl. Zero concentrations of C and O₂ are indicative to complete the conversion of C into CO and CO₂. The low concentration of CH₄ may be attributed to the high conversion of the steam reforming reaction.
as the carbon boundary point (CBP), the point where carbon is depleted. Similar trends and CBP have been reported by Pala et al. [3], Rabah [8], Rabah [13], Begum et al. [10], and Safarian et al. [34]. As $T_g$ increases, $H_2$ increases to a maximum point at $T_g \approx 760 \degree C$ and then slightly reverses downward. The decrease in the hydrogen content with increasing temperature is likely to be due to the shifting of the exothermic water gas shift ($CO + H_2O \leftrightarrow CO2 + H_2$) toward reactants. $CH_4$ is depleted with increasing temperature. $CH_4$ is produced by the C-methanation reaction and depleted by steam reforming relations. The same results have been observed for the remaining feedstock (not shown here).

Table 3: Optimization results.

<table>
<thead>
<tr>
<th>MSW</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
<th>11</th>
<th>Min</th>
<th>Max</th>
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</thead>
<tbody>
<tr>
<td>ER</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.01</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.01</td>
<td></td>
</tr>
<tr>
<td>SB</td>
<td>1.22</td>
<td>0.93</td>
<td>0.86</td>
<td>0.66</td>
<td>1.00</td>
<td>0.87</td>
<td>1.03</td>
<td>0.89</td>
<td>0.88</td>
<td>0.82</td>
<td>1.08</td>
<td>0.66</td>
<td>1.22</td>
</tr>
<tr>
<td>$T_g$</td>
<td>763</td>
<td>761</td>
<td>679</td>
<td>745</td>
<td>714</td>
<td>709</td>
<td>712</td>
<td>740</td>
<td>710</td>
<td>750</td>
<td>695</td>
<td>679</td>
<td>763</td>
</tr>
<tr>
<td>$\eta$</td>
<td>84.87</td>
<td>50.09</td>
<td>79.77</td>
<td>79.77</td>
<td>69.09</td>
<td>64.85</td>
<td>65.86</td>
<td>47.83</td>
<td>81.56</td>
<td>92.82</td>
<td>94.60</td>
<td>47.83</td>
<td>94.60</td>
</tr>
<tr>
<td>Y</td>
<td>1.02</td>
<td>0.51</td>
<td>1.21</td>
<td>1.17</td>
<td>1.09</td>
<td>0.97</td>
<td>1.09</td>
<td>0.71</td>
<td>1.32</td>
<td>1.39</td>
<td>0.73</td>
<td>1.73</td>
<td>1.73</td>
</tr>
</tbody>
</table>

Biomass % used as fuel for steam generation, drying, and pyrolysis

$\Delta s$ | 8.46| 7.16| 18.29| 17.10| 18.09| 17.90| 19.82| 17.78| 21.88| 18.58| 22.69| 7.16| 22.69|
$\Delta d$ | 2.98| 16.48| 4.87| 4.77| 8.09| 11.01| 8.77| 13.97| 4.95| 1.93| 0.38| 0.38| 16.48|
$\Delta p$ | 1.53| 4.11| 2.42| 1.94| 3.03| 3.42| 3.15| 1.38| 0.75| 1.28| 2.25| 0.75| 4.11|
$\Delta t$ | 12.98| 27.76| 25.58| 23.81| 29.21| 32.33| 31.74| 27.58| 21.79| 25.33| 12.98| 33.12|

Syngas compositions

$H_2$ | 58.67| 57.92| 53.03| 55.96| 54.01| 52.38| 53.63| 55.49| 54.05| 54.86| 55.51| 52.38| 58.67|
$CH_4$ | 6993| 5336| 29620| 6585| 9679| 8238| 9526| 5347| 10038| 3355| 29784| 3355| 29784|
$H_2O$ | 6.28| 6.28| 6.29| 6.28| 6.29| 6.29| 6.29| 6.28| 6.28| 6.28| 6.28| 6.28|
$N_2$ | 0.58| 0.38| 0.43| 2.33| 0.56| 0.96| 0.87| 0.45| 0.07| 0.50| 0.10| 0.07| 2.33|
$O_2$ | 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00|
$H_2S$ | 2814| 1674| 942| 1210| 2456| 2683| 2438| 305| 747| 221| 57| 2814|
$HCL$ | 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00|
$S$ | 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00|
$Cl_2$ | 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00| 0.00|
$C$ | 2.15| 2.15| 2.15| 2.15| 2.15| 2.15| 2.15| 2.15| 2.15| 2.15| 2.15| 2.15|

Syngas thermophysical properties

$\rho$ | 0.50| 0.52| 0.59| 0.54| 0.59| 0.62| 0.59| 0.57| 0.59| 0.58| 0.54| 0.50| 0.62|
$MW$ | 13.06| 13.52| 15.26| 14.14| 15.28| 16.06| 15.43| 14.71| 15.37| 15.05| 14.08| 13.06| 16.06|

3.4.2. Influence of SB on Syngas Quality. Figure 3(a) shows the influence of SB on CO, CO$_2$, $H_2$, and $CH_4$ mole fraction at constant ER and $T_g$. CO and $CH_4$ mole fractions are decreasing, while CO$_2$ and $H_2$ mole fractions are increasing with increasing SB. As SB increases, steam will be available for water gas shift and steam reforming reactions to convert CO and $CH_4$ into CO$_2$ and $H_2$ (see Table 1). The point where CO and CO$_2$ crossover is known as the carbon boundary point (CBP), as mentioned earlier. Figure 3(b) shows LHV, efficiency, and $H_2/CO$ versus SB. $H_2/CO$ decline is continuous, similar to the $CH_4$ profile. The decline in $H_2/CO$ is due to the increasing formation of CO. Excessively high gasification temperature ($T_g \geq 1000 \degree C$) tends to reduce the $H_2/CO$ molar ratio, LHV, and increase energy consumption, tar, and NO$_x$ formation.
assumes a positive linear variation with SB. At SB = 1.0, maximum efficiency and $H_2/CO \geq 2$ occur, which is consistent with optimization results.

3.4.3. Influence of ER on Syngas Quality. Figure 4(a) shows the influence of ER on the CO, CO$_2$, H$_2$, and CH$_4$ mole fractions at constant SB and $T_g$. The H$_2$, CO, and CH$_4$ mole fractions are decreasing with increasing ER, but CO$_2$ is increasing. This is expected, as more O$_2$ is available, complete combustion occurs, converting C to CO$_2$. CO and CO$_2$ crossovers occur at ER = 0.25. Similar trends have been reported by Pala et al. [3], Rabah [8], Begum et al. [10], and
Safarian et al. [34]. Figure 4(b) shows LHV, efficiency, and H₂/CO versus ER. Clearly, as more O₂ is available and the process is complete combustion and not biomass gasification process, it can be concluded that pure air gasification does not produce syngas quality that meets the FT synthesis requirement of H₂/CO ≥ 2.15. In addition, air gasification increases energy consumption and N₂ in syngas [31].

4. Conclusion

This work reports the results of the optimization model of biomass gasification, aimed to produce syngas for use as a feedstock for FT synthesis. The model is accomplished using the optimization section of the Model Analysis Tools of the Aspen Plus simulator. The thermal efficiency is maximized under the constraint of H₂/CO ≥ 2.15 molar ratio and the variables of SB = 0.0-5.0, ER = 0.0-1.0, and T_p = 500-1000°C. The simulation model is validated with the results obtained from the literature. The performance measures considered are syngas quality, thermal efficiency, LHV, and H₂/CO≥ molar ratio. The optimum operating conditions and syngas quality for eleven (11) types of MSW are made available. The optimum operating conditions have been found as ER = 0, SB = 0.66-1.22, and T_p = 679-763°C. Under the optimum operating conditions, a high-quality syngas has been produced with characteristics of H₂ = 52.38 -58.67%v/v and N₂ = 0.38-2.33%v/v, H₂/CO ≥ 2.15, and LHV = 12.55-17.15 MJ/kg, and zero NOx formation. The reported generalized optimization model is applicable to all types of biomass and coal.

Nomenclature

**Roman Letters**

AFR: Stichometric air-fuel ratio

Cᵦ: Isobaric specific heat capacity (kJ/kg K)

DAF: Dry and ash-free basis

E: Relative error

ER: Equivalence ratio

FC: Fixed Carbon

h: Enthalpy (kJ/kg K)

HHV: Higher heating value (MJ/kg)

LHV: Lower heating value (MJ/kg)

M: Mass flow rate (kg/s)

max: Maximum

min: Minimum

MSE: Mean square error

MSW: Municipal solid waste

MW: Molecular weight (kg/kmole)

RMSE: Root mean square error

_\dot{Q}: Heat transfer rate

SB: Steam to biomass ratio

toe: Ton of oil equivalent

T: Temperature (°C)

VM: Volatile matter

y: Gas mole fraction

Y: Yield

**Greek Letters**

\( \eta \): Thermal efficiency
Δ: Biomass % used as fuel for steam generation, drying, and pyrolysis (%)
λ: Latent heat of vaporization (kJ/kg)
ω: Moisture fraction.

Subscripts
b: Biomass
d: Drying
i: Index 1,2,3,..., input
p: Pyrolysis
o: Output
s: Steam
t: Total
w: Water
v: Vapor.

Superscript
°: Degree.

Data Availability
All information used to support the findings of the study are available from the corresponding author upon request.

Disclosure
The author conducted this work as part of his normal research activities as a professor of Chemical Engineering at the University of Khartoum, Sudan.

Conflicts of Interest
The author declares that he has no conflicts of interest.

References


