Simulation of biomass and municipal solid waste pellet gasification using Aspen Plus

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Abstract. The work deals with the simulation of biomass and municipal solid waste pellet gasification using Aspen Plus software. The effects of key parameters on the composition of the emitted gas are discussed, including gasification temperature, moisture content, and equivalence ratio. The sensitivity analysis was studied with the Aspen Plus Software, which includes FORTRAN modules. The simulation is validated using experimental results, which revealed that it was roughly correct. Using air as the gasification agent, the sensitivity analysis findings confirm higher temperatures promote syngas production with increased hydrogen and energy content. The simulation results demonstrated that CO\textsubscript{2} concentration (3.95\%) increases from 450°C to 600°C and then decreased drastically near 0.225kmol/hr. at 900°C. As the gasification temperature rises from 450°C to 900°C, the CO concentration rises and the H\textsubscript{2}: CO ratio falls. At 900°C, increasing the gasification temperature results in a product gas with more H\textsubscript{2} (65\%) and CO (12.43\%), resulting in a higher calorific value, whereas the contents of CH\textsubscript{4}, CO\textsubscript{2}, and H\textsubscript{2}O followed an inverse correlation. CH\textsubscript{4} decreased with temperature because of the formation of exothermic methane reactions. When the gasification process reaches 800°C, all components except CO\textsubscript{2} become steady, and gasification reactions were achieved. The equivalence ratio (ER) ranged from 0.2 to 0.3. The gas produced by a gasifier is highly dependent on the ER value. The ER determines the gas quality, and it must be less than 1 to ensure that it gasifies the fuel rather than burnt. Moisture content was 10wt. %, this is an essential parameter for the optimum conditions during the gasification process. Moisture content determines the gas characteristics at the exit phase. The model predictions and calculated values are in good agreement.

1. Introduction

The world's growing energy demands, as well as the production of a large amount of biomass waste, have fueled the development of biomass gasification technology [1]. Furthermore, the lack of fossil fuels and environmental problems such as greenhouse gas emissions, deforestation, and other health-related issues, is driving the hunt for alternative energy sources.

To replace fossil fuel, it is necessary to find alternative energy sources that are abundant, inexpensive, and have a low environmental impact. Biomass was suggested as a solution to these problems because it is green, easy to find, and long-lasting. The amount of CO\textsubscript{2} absorbed from the
atmosphere during photosynthesis of green biomass is nearly equal to the CO$_2$ produced during biomass combustion [2].

Gasification of municipal solid waste (MSW) and biomass waste offers significant opportunities for energy security and climate change mitigation. To avoid pollution of the environment due to waste accumulation, some developed countries encouraged the conversion of municipal solid waste into energy [3]. Thermochemical conversions such as combustion, pyrolysis, and gasification, as well as anaerobic digestion, were used to convert MSW to energy. The appropriate gasification operating parameters are also investigated, including gasification temperature, moisture content, and equivalence ratio. For this objective, a simulation model is developed, and the results are compared to published experimental data [4,5].

This study presents the gasification of the mix of MSW and empty fruit bunch (EFB) using the Aspen Plus simulator. The aim of this study was to use Aspen Plus to predict the impact of key variables on gasification, such as temperature, the equivalence ratio, moisture content, and syngas caloric value).

2. Methodology

2.1. Development of a Gasification Model

The Aspen Plus gasification model was used to transform a mixture of municipal solid waste and biomass waste feedstock into refuse-derived fuel pellets using a solid-based simulation. The following steps are involved in the development of a model in the simulator: The definition of the process flow-sheet, the description of the stream class, the choice of the property approach, the configuration of software packages (via a database), and the identification of conventional and non-conventional components (via unit operation blocks and linking material and energy flows) [6].

The gasification process includes drying (lowering the moisture content of fuel to 10% prior to supplying it to the reactor), pyrolysis (the raw material was decomposed into volatile compounds and char), and then gasification occurs.

2.2. Model assumptions

The following are the model’s fundamental assumptions:

1. Free kinetic model with a steady-state.
2. The (MSW+EFB) particles are a uniform size and temperature.
3. The model contains only ideal gases. To reduce the hydrodynamics complexity the influence of tar and other heavy products is not considered.
4. All sulfur is converted to H$_2$S.
5. There are no nitrogen oxides produced, only NH$_3$, [1, 7].

Table 1 depicts the models of ASPEN Plus unit operation.

| ASPEN PLUS ID | ID of the block | Description |
|--------------|----------------|-------------|
| RStoic       | DRIER          | Reduces the fuel's moisture content |
| RYield       | DECOMP         | Yield reactor- uses FORTRAN statements to convert non-conventional biomass into conventional components. |
| RGibbs       | GASIFIER       | Gibbs free energy reactor: By reducing Gibbs free energy, this reactor deals with three-phase equilibrium and estimates synthesis gas mixture. |
| Sep          | SEPARATOR      | Split fractions are used to remove gases from ash. |

2.3. Physical property method

The PR-BM property approach was used for the Peng-Robinson (PR) equations. The Boston-Mathias (BM) alpha formula is used in the PR-BM property method to measure physical properties of the conventional components in the gasification.
The temperature-dependent variable alpha is included in this property package. Hydrocarbons and light gases like carbon dioxide, hydrogen sulphide, and hydrogen are examples. This property approach is very useful in high-temperature, high-pressure environments, such as hydrocarbon processing or supercritical extractions. HCOALGEN and DCOALIGT were used as the enthalpy and density models for the non-conventional components (MSW, biomass, and ash).

2.4. Description of the Model

The gasification process simulation model was created on Aspen Plus software using three (3) main reactor types: Stoichiometric Reactor (RStoich), the Yield Reactor (Ryield), and the RGibbs Reactor. The process steps are illustrated in Figure 1. The mixture (Biomass and MSW) is developed in the simulation model utilizing the proximal and ultimate analyses and is specified as a non-conventional component in ASPEN Plus.

Table 2 contains the data used to describe the feedstock. The 'RStoic' block was used to simulate the drying process (MW and biomass). Evaporation is used in this phase to reduce the moisture content of the feedstock. Furthermore, the drying process has been regulated by asserting in a calculator block and describing the raw material drying process using FORTRAN modules. To all non-conventional elements, Aspen assigns a molecular weight of 1. The entire production of volatiles is assumed to be equal to the parent fuel's volatile content, whereas the average production of carbonaceous materials is proportional to the carbon content and ash concentrations calculated through proximate analysis.

Biomass particles are heated to 100-150 °C in a gasifier, dried, and the moisture is removed as steam. Because gasification is an endothermic reaction, heat is delivered to the particle, which is heated to 500 °C, knocking off all volatiles. During this process, approximately 70-80% of the dry biomass weight is lost. Char is the solid biomass that is left over after the combustion process. In the presence of heat and a medium agent, this char gasifies, releasing the second collection of gases. After the drying stage, the decomposition process model (Ryield block) begins, converting non-conventional feed components, in this case, a mixture of (MSW) and biomass, into conventional compounds (C, H, N, O, S, and ash). This is accomplished by employing the RYield model and performing calculations in the calculator block based on part output stipulations (FORTRAN). Because it takes less time and releases around 80-90% of the mass as steam, devolatilization is a significant step in gasification. Unlike pyrolysis, gasification focuses on boosting gas output. As a result, the operating conditions for gasification have been improved to allow the release of volatiles from biomass [8].

The converted elements are ready for gasification after decomposition. Furthermore, in this block, the air stream introduces air or steam as a medium. The RGibbs reactor model, which is rigorous and can measure chemical and phase equilibrium by minimizing the system's Gibbs free energy, is used to simulate this gasification step. The emitted gas passes through another separator block to extract the ash as slag from the GASIFIED stream as it exits the reactor (SEP2).

The RGibbs reactor receives the decomposed biomass and air, which undergoes partial oxidation and gasification reactions. H2S is formed when all of the sulfur in the feedstock reacts with H2. Because of the low sulphur content of fuel, the discrepancies of this simplification are negligible.

Other researchers [9-12], have assumed that just NH3 is formed and no nitrogen oxides are generated. The unit activity model Sep was used to simulate the separation of ash from syngas. The RGibbs reactor's outlet stream enters the Sep block, which uses split fractions to separate gases from ash. Figure 1 depicts the Aspen Plus process flow for municipal and biomass mixture gasification.
Figure 1. Aspen Plus process flow for municipal and biomass mixture gasification.

The analysis of feedstock conditions at the ultimate and proximate levels as well as the gasification process operating parameters are shown in Tables 2 and 3.

Table 2. Analysis of Feedstock Conditions at the Ultimate and Proximate Levels.

|                         | Municipal solid waste + Empty fruit bunch |
|-------------------------|------------------------------------------|
| Proximate analysis (mass %) | Ultimate analysis (mass %)              |
| FC                      | 85.02                                    |
| VM                      | 2.53                                      |
| MC                      | 8.23                                      |
| ASH                     | 4.22                                      |
| C                       | 52.50                                     |
| H                       | 7.95                                      |
| O                       | 34.91                                     |
| N                       | 0.33                                      |
| S                       | 0.07                                      |

Table 3. Gasification Process Operating Parameters.

| Parameter                  | Value  | Unit   |
|----------------------------|--------|--------|
| Feed rate                  | 1000   | Kg/h   |
| Steam/ biomass ratio       | 0.5-1  |        |
| Feed Temperature           | 25     | ºC     |
| Feed Pressure              | 1      | atm    |
| Air Pressure               | 1      | atm    |
| Air Temperature            | 25     | ºC     |
| Gasifier Temperature       | 450-900| ºC     |
| Gasifier Pressure          | 1      | atm    |

2.5. Validation of the model

Three sets of experimental results from pilot-scale fluidized bed gasification processes published in the literature were used to validate the simulation results. The design can forecast gasifier efficiency under a variety of conditions, such as temperature, and equivalence ratio, among others.

3. Results and Discussions

In general, there are two types of gasification processes. Basic pyrolysis is the early stages, which involves dissolution of municipal solid waste to generate gases, ash, and char. In the second phase, homogeneous and heterogeneous reactions take place in a reducing atmosphere [13].

As a function of gasification temperature, Figure 2 shows the generated gas molar fraction. The actual content of the output will be influenced by the temperature of the gasifier. Le Chatelier’s principle states that higher temperatures favor endothermic reaction products. Endothermic reactions occur in a number of significant reactions within the gasifier. Moreover, as shown in Figure 2,
increasing the combustion temperature results in the production of produced gas with increased H2 and CO concentrations, and hence a calorific value. The contents of CH4, CO2, and H2O follow the opposite result, with CH4 decreasing with the temperature due to the exothermic nature of methane reactions. Furthermore, at 800 °C as the gasification temperature, all components except CO2 become stable, and the gasification reaction tends to complete. The findings show that as the temperature rises from 450 °C to 650 °C for H2, the contents of Hydrogen and CO enhance. As a result, two reactions (R1) and (R2) increase H2, while (R3) and (R4) increase CO. The research results are similar to those reported in [14, 15].

Figure 2. The influence of temperature on syngas composition.

Higher temperatures promoted hydrogen production and gas yield in general, but not always gas heating value, as too high a temperature decreased gas heating value. The quality of syngas degrades as moisture content rises, and gasifier temperatures have been found to have a greater impact on syngas composition [16]. Endothermic reactions, such as the Boudouard reaction, the water gas reaction, and steam methane reforming, prefer forward reactions as the gasification temperature rises.

C+ 0.5O2 ↔ CO –111 MJ/kmol Partial oxidation R1
C+ H2O ↔ CO +H2 +131MJ/kmol Water gas reaction R2
CO+H2O ↔ CO2 – 41MJ/kmol water gas shift R3
C+CO2 ↔ 2CO +172MJ/kmol Boudouard R4
C+ 2H2 ↔ CH4 – 74MJ/kmol methanation R5

Figure 3 demonstrates the effect of temperature on hydrogen and CO ratio.

As the gasification temperature increases, the H2: CO ratio drops (refer to Figure 3). According to [17], the steam to biomass ratio (SBR) is an important process factor in the gasification of steam. The fundamental benefit of using steam as an agent is that it enriches the molecular fraction of H2 and increases the concentration of H2O, resulting in more water shift reactions.
Figure 4. Effects of ER on the composition of syngas.

Suitable temperature range for a maximum amount of H$_2$ and CO is 650 to 900 °C. There is a similar variation between CO$_2$ and H$_2$O. Moreover, the equivalence ratio (ER) and steam biomass ratio (SBR) rise with the CO$_2$ and H$_2$O increase. CO$_2$ increases with temperature to a maximum value at 550 °C and later starts decreasing. While H$_2$O decreases, with an increase in temperature, reaches its minimum value at 650 °C, and next starts increasing. CO$_2$ and H$_2$O reach their peak at the same temperature interval. Increased ER speeds up the oxidation reaction and lowers the quality of product gas. A high ER, on the other hand, results in low H$_2$ and CO concentrations in the product gas, as well as a high CO$_2$ content. [18, 19] investigated the effect of ER on biomass air gasification in a fluidized bed gasifier from 0.15 to 0.35, and from 0.1 to 0.9 [1]. They discovered that as ER increased, H$_2$ and CO increased at first and then decreased, whilst CO$_2$, CH$_4$, and other hydrocarbons’ content was gradually reduced, which is similar to our findings. Table 4 depicts a comparison of modeling and experimental results.

Table 4. A comparison of modeling and experimental results.

| Temperatures | Gas composition | vol% | Error % | vol% | Error % | vol% | Error % | vol% | Error % |
|--------------|-----------------|------|---------|------|---------|------|---------|------|---------|
| 550°C [18]   | H$_2$ Simulation| 53.34| 1.94 | 65.47| 4.14 | 66.14| 1.75 | 65.07| 1.21 |
|              | H$_2$ Experiment| 54.4 | 68.3 | 65   | 65.87 |
| 650°C [18]   | CO Simulation | 4.19 | 7.43 | 9.37 | 14.8 | 11.19| 15 | 12.43| 12.8 |
|              | CO Experiment | 3.9 | 11 | 14 | 14.26 |
| 750°C [5]    | CO$_2$ Simulation | 6.31 | 7.86 | 5.46 | 16.51 | 4.26 | 19.3 | 3.06 | 4 |
|              | CO$_2$ Experiment | 5.85 | 6.54 | 5.28 | 3.2 |
| 900°C [6]    | CH$_4$ Simulation | 4.99 | 9.27 | 0.66 | 20 | 0.004 | 20 | 0.001 | 50 |
|              | CH$_4$ Experiment | 5.5 | 0.55 | 0.005 | 0.002 |

By comparing the composition of the product gas generated from this work’s constructed model to the data published in the literature by [5-6,18] the gasification model was validated. At the gasification temperatures of 550, 650, 750 and 900 °C, the mole fractions of gas product were compared. Our simulation results, as shown in Table 4, are comparable to literature values, and the main component errors are low, except CH$_4$. This implies that the chemical equilibrium model established in this study is reliable and can be used to simulate the gasification of MSW and EFB mixtures.

4. Conclusion
Variations in gasifier temperature, ER, and moisture content were tested to see how they affected syngas composition, HHV, and hydrogen generation. As the temperature of the gasifier rises, so does the generation of carbon monoxide and hydrogen. Higher moisture content affects the HHV and degrades gasifier performance. The simulation results were validated using three sets of experimental data from pilot-scale fluidized bed gasification systems described in literature. In the current investigation, the resultant syngas has a substantially larger mole fraction of H$_2$ than CO, and the...
operating conditions are very comparable to the results being refered. The major changes are found in the parameters of the raw material, specifically the moisture content (10 wt.%) and (12-48 wt %) in the other studies. It also has very similar working conditions to those from previous studies. The model predictions and the calculated values were in good agreement.

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