Simplified gasification simulation using zero-dimensional model of empty palm fruit bunch

P N A Nugroho 1 and S Torii 2

1Politeknik Perkapalan Negeri Surabaya, Jl. Teknik Kimia, Kampus ITS Sukolilo, Surabaya 60111, Indonesia.
2Department of Advanced Mechanical System Engineering, Kumamoto University, Kurokami, 2-39-1, Kumamoto 860-8555, Japan

priyambodo@ppns.ac.id

Abstract. As one of the most efficient biomass conversions, the gasification process is hard to understand because of its complexity. A simplified gasification process simulation using a zero-dimensional model was designed for an empty fruit bunch considering its potential in Indonesia. A stoichiometric equilibrium model was applied to simulate the whole gasification process. Global gasification reaction, mass, and energy balance with two independent chemical reactions are integrated to perform the model. Some sets of linear and nonlinear equations were solved with the Newton Raphson method in Matlab. The output of the model, like syngas composition and the heating value, was validated with available experimental data published. The zero-dimensional thermodynamic equilibrium model could be used to predict the maximum performance of the gasifier and make the gasification process more feasible.

1. Introduction
Palm oil has been used for centuries ago. Originally from Africa, palm tree (Elaeis guineensis) has been naturalized in tropical countries since it grows even better. Palm tree produces crude palm oil (CPO) that could be used in a vast range from cooking oil to biodiesel. CPO become an internationally traded community and is very important for Indonesia as the largest CPO producer.

Along with Malaysia, over 20 million metric tons of CPO produced in the almost 10-million-hectare area. Maitah et al. reported that CPO production also generates a large amount of biomass [1]. For every 1 kg of CPO, about 4 kg of biomass waste. Most of the waste is an oil palm empty fruit bunch; the other is fronds and trunks.

Gasification is the thermochemical process that converts carbonaceous material like coal or biomass into valuable gaseous fuel or chemical substance. The history of Gasification could be traced back to 1659 when Thomas Shirley discovered gas from a coal mine. In 1739 Dean Clayton successfully distilled coal in a closed vessel followed by Robert Gardner patented its first gasification technique in 1788. According to Basu, biomass intended not only energy conversion but also the production of a chemical substance as one of the essential commodities [2].

Similar to Gasification, combustion also changes carbonaceous material into product gases. However, there is distinctness like there is no useful heating value in the combustion product gas, in contrast to Gasification that possesses beneficial heating value. Combustion release energy in its process, while Gasification packs energy into compact chemical bonds. The combustion process...
occurred in an oxidizing environment and releasing heat, while Gasification happened in inadequate oxygen surrounding and demanding heat.

The gaseous medium of Gasification is involved in the process of converting either fossil or non-fossil fuel into valuable gaseous fuel or other chemicals. Gaseous mediums example is oxygen, air, steam, or a mixture of them. The reason behind transforming potential fuel into another form is to increase the heating value of the fuel by releasing non-combustible matter like nitrogen and water. Another motivation is to remove sulphur and nitrogen from the fuel so that this material will not be released into the atmosphere when burning the fuel. An additional motive is to reduce the proportion of carbon to hydrogen ratio in the fuel.

Generally speaking, the more hydrogen contents in the fuel, the lower the vaporization temperature and increases the likelihood of fuel become in the gaseous phase. Biomass gasification converts solid-state biomass into gaseous state fuel or chemicals. The chemical energy contained in the solid biomass is changed into the thermal and chemical energy of the gas. Hence the chemical energy within the product gas is a function of its chemical configuration. In other words, the quality of the product is driven by chemical composition. Htut et al reported that the outcome of Gasification is called the syngas in which CO and H2 are the main gaseous species [3].

Forecasting performance using thermodynamic computations are commonly used to explain chemical reactions within the gasifier. Performance prediction of a downdraft gasifier has been made by Zainal et al using equilibrium modelling for some biomass materials like wood, paddy husk, paper, and municipal waste [4]. It was found that the heating value of the syngas decrease along with increasing gasifier temperature and also an increase in moisture content.

Wu and Chein have worked on the modelling of biomass gasification with high-temperature inlet as a result of preheating [5]. Combustible species reduction was acknowledged with more than a certain amount of biomass moisture content. Preheated air could enhance gasifier performance; however, the degree of significance was lower than expected.

Align with the great curiosity about the biomass gasification process and make the process more feasible. It is inevitable to model and foresee the gasifier performance before building the actual one. This paper aims to perform syngas composition and heating value analysis composed of the gasifier with a zero-dimensional equilibrium model.

2. Materials and Methods

The gasification process designed in this paper is illustrated in Figure 1. Biomass enters the gasifier at temperature $T_b$, while air as the gasifying agent has temperature $T_a$ and pressure $P_a$. Temperature and pressure inside the gasifier are $T_g$ and $P_g$, respectively. Syngas formed, leaving the gasifier at temperature $T_s$ and pressure $P_s$.

![Figure 1 Gasification Process Illustration](image)
Some assumptions, according to Wu and Chein [5] and Htut et al. [3], were taken into consideration to simplify the analysis.

- The thermodynamic equilibrium process and adiabatic (no heat transfer from and to the environment) happens in all gasification reactions.
- Thermodynamics properties like temperature, pressure, and species concentration are uniformly distributed within the gasifier.
- Steady-state condition is already achieved within the gasifier.
- Biomass from palm empty fruit bunch expressed as CHₐOₜₙ. a, b, and c are the number of atoms of hydrogen, oxygen, and nitrogen, respectively, derived from the ultimate and proximate analysis in table 1.
- There is no solid carbon remaining after the gasification. All converted into syngas species in the global gasification model.

**Table 1. Empty Fruit Bunch Ultimate and Proximate Analysis [5]**

| Component   | %(Wt) | Element | %(Wt) |
|-------------|-------|---------|-------|
| Volatile    | 77.46 | C       | 61.51 |
| Fixed Carbon| 17.25 | H       | 10.51 |
| Ash         | 5.29  | O       | 26.00 |
|             |       | N       | 1.98  |

- Syngas produced from the gasification process is consisting of H₂O, N₂, H₂, CO, CO₂, and CH₄. Ideal gas law applied to all of the syngas.

Model input required the following information:

- Biomass chemical composition (CHₐOₜₙN_c), biomass, and initial air temperature derived from the ambient temperature.
- Average gasification equilibrium temperature ranging from 800 to 1000 °C.
- An equilibrium constant (K) used in gasification reaction is from methane forming and water gas shift reaction.
- Thermodynamic data for a chemical substance in gasification reactions like enthalpy for formation (H°f) and specific heat (C_p) taken from Perry [6].

Model output is the syngas composition once the equilibrium state achieved and the syngas heating value calculated from the syngas composition. Syngas heating value could be determined from bomb calorimeter, but also could be estimated with the calculation proposed by Reed [7].

\[
\Delta H_c = LHV \ (kJ/kg) = 0.2326(146.58C + 56.878H - 51.53O - 6.58A + 29.45) \quad (1)
\]

Where C, H, O, and A are the mass fractions of carbon, hydrogen, oxygen, and ash, respectively, in the dry biomass.

Global biomass gasification for solid biomass CHₐOₜₙN_c with air as gasification agent could be written with equation (4) below

\[
CH_{a}O_{b}N_{c} + wH_{2}O + m(O_{2} + 3.76N_{2}) \rightarrow n_{1}H_{2} + n_{2}CO + n_{3}CO_{2} + n_{4}H_{2}O + n_{5}CH_{4} + n_{6}N_{2} \quad (2)
\]

Where the amount of water per kmol of biomass is denoted as w, and the amount of oxygen per kmol of biomass is indicated as m. The remaining coefficient of a constituent of products is marked as n₁₋₆. w could be calculated from moisture content per mol of biomass, so w become constant once moisture content was identified.

Mass balance is used from the atomic species balance to express the constraints of the gasifier system
\[ C: 1 = n_2 + n_3 + n_5 \]  
\[ H: 2x + a = 2n_1 + 2n_4 + 4n_5 \]  
\[ O: b + x + 2y = n_2 + 2n_3 + n_4 \]

Two independent reactions (methane formation and water gas shift reaction) were used to model independent reactions, the case of reactions without the presence of unconverted carbon in the products.

\[ C + 2H_2 \leftrightarrow CH_4 \; \text{and} \; K_1 = \frac{x_5}{x_2^2} \]  
\[ CO + H_2O \leftrightarrow CO_2 + H_2 \; \text{and} \; K_2 = \frac{x_3^2 x_4}{x_1 x_2} \]

The equilibrium constant for each reaction is expressed as \( K_1 \) and \( K_2 \), which is the function of temperature.

The last constraint is the energy balance as one of the essential equations that occurred in the adiabatic process without the transfer of heat or mass of substances between the thermodynamic system and surrounding. Energy is transferred to the surroundings as work only.

\[ H^0_{f,bio} + w(H^0_{f,H_2O(l)} + H_{(vap)}) = n_2H^0_{f,CO} + n_4H^0_{f,H_2O(vap)} + n_5H^0_{f,CH_4} + \Delta T(n_1C_{PH2} + n_2C_{PCO} + n_3C_{PCO2} + n_4C_{PCH2} + n_5C_{PCH4} + 3.76y_{CPN2}) \]  

In summary, there are six unknown parameters \((n_{1,6})\) and six independent relations; three relations from the mass balance reactions (equation 5, 6 and 7), two relations from independent chemical reactions (equations 8 and 9), and one relation from energy balance (equation 10).

Substitutions and eliminations were used on the mass balance, energy balance, and independent reactions to solve the composition of carbon, hydrogen, and oxygen.

After going through the calculation steps, the constant equilibrium \( K_1 \) and \( K_2 \) for any particular temperature \( T \) could be calculated with following general equation for \( K_1 \) and \( K_2 \)

\[ \ln K_1 = \frac{7082.848}{T} - 6.567 \ln T + \frac{7.466 \times 10^{-3}}{T^2} - \frac{2.164 \times 10^{-6}}{T^2} + 0.701 \times 10^5 \times 10^{-3} \times 10^{-6} + 32.541 \]  
\[ \ln K_2 = \frac{5872.46}{T} + 1.86 \ln T - 2.69 \times 10^{-4} T + \frac{58200}{T^2} - 18.0139 \]

The remaining equations were consisting of linear and nonlinear equations and solved with the Newton Raphson method and fsolve in Matlab.

Biomass gasification performance could be indicated using some indicators. In this paper, syngas composition and LHV are used to indicate the gasification performance. Syngas composition was calculated from equation (11) and (12), while LHV or the Lower Heating Value of biomass could be found from equation (1), reference [4], and [8]. Gasification temperature and ER were varied to achieve the best gasification performance.

3. Result and Discussion

The results were validated with some previously developed models, analytical, numerical, and experimental models. Root Mean Square Error (RMSE) analysis method was employed to verify which model was better.

\[ RMSE = \sqrt{\frac{\sum_{i=1}^{N}(y_{Exp} - y_{Model})^2}{N}} \]  

\[ i = 1 \]
Table 2 shows a comparison between the zero-dimensional model (A) and some available data from the literature. As seen in Table 2, The proposed model (A) has lower RMSE compared with other research published (A1), hence in comparison with experimental data; therefore, the zero-dimensional method was relatively close with actual data.

|         | A1  | A   | E   |
|---------|-----|-----|-----|
| H₂ (%)  | 14.00 | 14.95 | 17.50 |
| CO (%)  | 20.14 | 20.85 | 21.30 |
| CH₄ (%) | 12.06 | 16.85 | 13.30 |
| CO₂ (%) | 2.31  | 2.01  | 3.10  |
| N₂ (%)  | 50.79 | 45.91 | 44.20 |
| LHV (MJ/m³) | 5.28  | 5.01  | 5.69  |
| RMSE    | 3.44 | 2.16 |     |

All the models show a good agreement with the experimental data, with syngas composition from the highest to the lowest fraction, which is N₂, CO, CH₄, H₂, and CO₂, respectively. Hence the proposed model could be justified because RMSE evaluates the discrepancy between values provided by the model and the observed value from the experimental analysis.

The goal of gasification modelling is to achieve a maximum heating value from syngas. Syngas further usage following the Gasification should also be considered. According to Htut, syngas for the internal combustion engine usage will require heating value more than 4.2 MJ/m³ [3]. All of the models and experimental data already meet this requirement.

The effect of gasification temperature on the heating value could be seen in Figure 2. The maximum heating value could be achieved with gasification temperature range 800-900 °C, or it could be concluded that within the gasification range 800-900 °C maximum syngas fraction of hydrogen, carbon monoxide, and methane was achieved.

![Figure 2. Effect of Gasification Temperature and ER](image)

Equivalence Ratio (ER) variation also affects the Heating Value of syngas produced by the gasifier. Lower ER ratio tends to have lower heating value, an increase from 0.1 to 0.2, and reach the maximum heating value at ER 0.3. Higher ER value resulting in a drop in heating value compared to 0.3
4. Conclusions
Gasification simulation models could be classified based on the spatial dimension from the complicated three-dimensional models to the simple one-dimensional model. A zero-dimensional equilibrium model was established and proven its reliability with the experimental data. Thermodynamic computations are unconstrained with the dimension of the gasifier; hence it is advantageous to analyse the most substantial process parameters.

This model could be used to predict the gasification performance parameter (syngas composition and heating value) with satisfactory precision — the fact that both pyrolysis and syngas products were all need to go through the oxidation zone or the highest temperature in the gasifier. Equilibrium phase could be achieved even in a brief time in the oxidation zone. The advantage of this model is that this model could be able to manage a wide range of biomass sources of materials with different operating conditions and quite simple to operate.

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