



Modelling and Optimisation of Gasification for Palm Kernel Shell (PKS) in a Fluidized Bed Gasifier

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In line with human population growth, the demand for energy has increased drastically. As the world is soon facing the shortage of fossil fuels, production of biofuel from biomass has been identified as one of the most promising alternative renewable energy sources to support the energy demand. As biomass gasification can convert variety of biomass feedstock into syngas which can be used as feedstock for the production of liquid fuels and chemicals as well as the generation of heat and power; therefore, biomass gasification is recognised as a promising first processing step in an integrated biorefinery. In this work, modelling based on the experiment results of a fluidised bed gasifier is presented. Palm kernel shell (PKS) is taken as the feedstock of the gasifier. Based on the developed model, the gasifier can be optimised to achieve various objectives, such as maximum hydrogen production. In addition, the composition of the syngas can also be determined.

1. Introduction

According to Malaysian Palm Oil Council (MPOC), Malaysian palm oil industry has become the second largest palm oil producer in the world, accounting for 39 % of world palm oil production and 44 % of world exports. The oil palm solid wastes (including palm kernel shell (PKS), empty fruit bunches (EFB), mesocarp fibers etc.) are discharged from the mill. Palm kernel shell is one of the best potential biomass feedstock available as it has high heating value of 24.97 MJ/kg (Esfahani et al., 2009).

Gasification process is one of the most promising thermo-chemical conversions of biomass to energy. Gasification typically operates in a temperature range of 600 °C – 1400 °C (Ciferno and Marano, 2002), with a controlled supply of oxygen and/or steam to convert biomass into as syngas which consists of carbon dioxide (CO₂), steam (H₂O), methane (CH₄), carbon monoxide (CO) and hydrogen (H₂). Syngas produced from biomass gasification through the robust thermal conversion can be used as feedstock for the production of liquid fuels and chemicals as well as the generation of heat and power. Biorefinery is a facility that integrates biomass conversion processes and equipment to produce fuels, power, and chemicals from biomass. To enhance the overall process and economic performances, the concept of integrated biorefinery, which integrates multiple platforms as a whole, has been proposed (Fernando et al., 2006).

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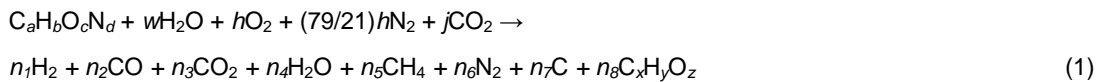
2. Literature Review

According to Li et al. (2001), gasification modelling is predominantly divided into two categories: kinetic modelling and thermodynamic equilibrium modelling. There are two methods for thermodynamic equilibrium modelling which are stoichiometric and non-stoichiometric equilibrium (Huang and Ramaswamy, 2009). The stoichiometric method is based on stoichiometric reactions while non-stoichiometric method is based on minimising the total Gibbs free energy in the system. It is noted that equilibrium models with or without char formation were widely studied. However, in the actual gasification system, equilibrium chemical reactions are hardly entertained due to kinetic limitations (Li et al., 2004). Therefore, the models were modified and calibrated by fixing the amount of syngas to value derived from experimental results with multiplying equilibrium constants (Barman et al., 2012). Modification of model was made to upgrade their equilibrium model to match experimental data and the results obtained were fairly agreeable with reference models taken. It is worth mentioning that the previous works were developed used a correction factor to modify the equilibrium constants in each reaction and limited to single temperature.

In this work, a stoichiometric equilibrium model of biomass fluidized bed gasifier is first developed. Next, the model is further improved by including correction factor to the equilibrium constants with a function of temperature. To ensure the accuracy of model, predicted syngas composition is then validated with the experimental results. Based on the developed model, the gasifier can be optimised to achieve various objectives, such as maximum hydrogen production. A case study with PKS as biomass feedstock is used to illustrate the approach.

3. Biomass Gasification Modelling

Biomass can be generally defined as $C_aH_bO_cN_d$ which can be determined from the ultimate analysis of biomass which gives the compositions of the biomass in weight percentage of carbon (C), hydrogen (H), oxygen (O) and nitrogen (N) (Jarungthammachote and Dutta, 2007). Based on the experiment conducted, other than syngas and solid carbon are produced by-products such hydrocarbons ($C_xH_yO_z$), tars, inorganic constituents, and ash are obtained throughout the experiment. The overall gasification reaction with air (79 % N_2 and 21 % O_2), steam (H_2O), and CO_2 can be written as (Tay et al., 2011):



where a , b , c , and d represent the number of atoms of C, H, O, N of biomass, respectively; w , h and j are the stoichiometric coefficients (per mole of biomass feedstock) of biomass moisture, oxygen, and carbon dioxide, respectively; $n_1 - n_7$ are the stoichiometric coefficients of H_2 , CO , CO_2 , H_2O , CH_4 , N_2 and solid carbon; x , y , and z represent the number of atoms of C, H, and O of hydrocarbons respectively; n_8 are the stoichiometric coefficient of hydrocarbons ($C_xH_yO_z$).

Based on Eq. 1, the atomic balances of C, H, O and N in biomass gasification are expressed as followed:

$$C: a f_i + j = n_2 + n_3 + n_5 + n_7 + x n_8 \quad (2)$$

$$H: b f_i + 2w = 2n_1 + 2n_4 + 4n_5 + y n_8 \quad (3)$$

$$O: c f_i + w + 2m + 2j = n_2 + 2n_3 + n_4 + z n_8 \quad (4)$$

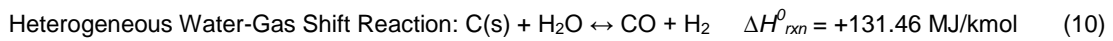
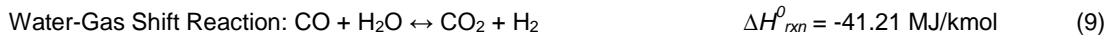
$$N: d f_i + (79/21)m = 2n_6 \quad (5)$$

where f_i is the molar flow rate of the biomass i .

As the main objective of this work is to predict and optimise the syngas composition without considering additional heat transferred into the gasifier, therefore, the enthalpy balance can be neglected. In this study, only mass balance and thermodynamic equilibrium equations are taken into account in modelling work. To further simplify the modelling efforts, the gasifier is assumed operating

under steady state conditions and atmospheric pressure. Other than that, syngas behaves as an ideal gas, whereas ash and N₂ are assumed to be inert at high temperature.

In a thermodynamic equilibrium model of gasification, five reactions that involve all chemical species are considered and shown in Eqs. 6 – 10. In this study, since solid carbon (i.e., ash) remains as a significant gasification product obtained in the experiment; therefore, the formation of solid carbon cannot be neglected. Three independent reactions are needed for the equilibrium calculations. Methane decomposition (Eq. 8), water-gas shift reaction (Eq. 9) and heterogeneous water gas-shift reaction (Eq. 10) are selected to represent the interaction of all components.



To determine the equilibrium constants by reaction temperature T , the standard free energy formation and the thermodynamic relation is expressed as:

$$K_{\text{MD}} = \exp(k_{\text{CO}} - k_{\text{H}_2\text{O}} - k_{\text{CH}_4}) \quad (11)$$

$$K_{\text{WGS}} = \exp(k_{\text{CO}_2} - k_{\text{H}_2\text{O}} - k_{\text{CO}}) \quad (12)$$

$$K_{\text{HWGS}} = \exp(k_{\text{CO}} - k_{\text{H}_2\text{O}}) \quad (13)$$

where $k_{\text{H}_2\text{O}}$, k_{CH_4} , k_{CO} and k_{CO_2} are the thermodynamic equilibrium constants for the formation reaction of H₂O, CH₄, CO and CO₂ at the reaction temperature T .

Based on the work of Baron et al. (1976), the $k_{\text{H}_2\text{O}}$, k_{CH_4} , k_{CO} and k_{CO_2} can be expressed by following equations:

$$\ln k_{\text{H}_2\text{O}} = 28780 T^{-1} - 0.69477 \ln T - 1.4283 \times 10^{-3} T + 0.74925 \times 10^{-6} T^2 - 1.3785 \times 10^{-10} T^3 \quad (14)$$

$$\ln k_{\text{CH}_4} = 8372.2 T^{-1} - 1.0769 \ln T - 5.6435 \times 10^{-3} T + 2.9046 \times 10^{-6} T^2 - 5.2351 \times 10^{-10} T^3 \quad (15)$$

$$\ln k_{\text{CO}} = 13612 T^{-1} + 1.8317 \ln T - 2.7584 \times 10^{-3} T + 0.6536 \times 10^{-6} T^2 - 0.78772 \times 10^{-10} T^3 \quad (16)$$

$$\ln k_{\text{CO}_2} = 47280 T^{-1} + 0.1322 \ln T - 0.94025 \times 10^{-3} T + 0.45112 \times 10^{-6} T^2 - 0.91901 \times 10^{-10} T^3 \quad (17)$$

However, the reactions might not interact ideally. As mentioned previously, models can be further modified by multiplying the equilibrium constants with correction factors ($\alpha_1 - \alpha_3$) to yield a corrected activity coefficient of reactants and products:

$$\alpha_1 K_{\text{MD}} = \frac{m_1^3 m_2}{m_4 m_5} P^2 \quad (18)$$

$$\alpha_2 K_{\text{WGS}} = \frac{m_1 m_3}{m_2 m_4} \quad (19)$$

$$\alpha_3 K_{\text{HWGS}} = \frac{m_1 m_2}{m_4} P \quad (20)$$

where K_{MD} , K_{WGS} and K_{HWGS} are equilibrium constants for methane decomposition, water-gas shift reaction and heterogeneous water gas-shift reaction, respectively; $m_1 - m_5$ is the molar fraction of H₂, CO, CO₂, H₂O, and CH₄; P is the operating pressure of the gasifier. To compare the predicted syngas composition from the modified model and experimental results, summation squared deviation method which also known as root-mean squared (*RMS*) is in used. The *RMS* is expressed as:

$$RMS = \sqrt{\frac{\sum_g (Exp_g - Mod_g)^2}{D}} \quad (21)$$

where g is syngas species, Exp is the value obtained from experimental result, Mod is the predicted result from the model, and D denotes number of syngas species considered in determining RMS .

4. Model Modification, Validation and Optimisation

The experimental data reported by Esfahani et al. (2012) was used as a base case of PKS. Based on the ultimate analysis, the empirical formulae of PKS is given as $CH_{1.283}O_{0.594}N_{0.031}$.

4.1 Determination of Correction Factor

As mentioned previously, in order to enhance the prediction of syngas composition for a specific type of gasifier, correction factor can be included. In this work, model is solved by inserting operating conditions and syngas composition (Esfahani et al., 2012) with the constraints in Eqs. 1 – 5 and 8 – 20 via Lingo 13.0 with Global solver to determine the correction factors (α_1 , α_2 and α_3).

4.2 Modification of Model

To further improve the accuracy of the model, the correction factors are taken as a function of temperature instead of a constant as in previous works. Such via modification, the model can predict the syngas composition more accurately in the given operating temperature range.

To determine the correction factors with function of temperature, different correction factors are first determined via Lingo 13.0 at different temperatures. Next, regression is conducted to determine the relationships between the correction factors with operating temperatures. To simplify the complexity of model, the outliers are removed for the analysis. The relationships between operating temperature and correction factors (α_1 , α_2 and α_3) of PKS is plotted. The regression analysis is performed via multiple regression in Microsoft Office Excel which performs both linear and exponential multiple regression analysis. An equation with higher value of R^2 is chosen to represent the relationship between two variables. The relationship of temperature and correction factors for PKS is written as:

$$\alpha_1 = \exp\left(\frac{146.81 - T}{128.1}\right) \quad (22)$$

$$\alpha_2 = \exp\left(\frac{T - 1116.7}{131.39}\right) \quad (23)$$

$$\alpha_3 = \exp\left(\frac{317.92 - T}{197.4}\right) \quad (24)$$

Note that there are total eleven unknowns ($n_1 - n_8$) and only seven equations (Eqs. 2 – 5 and 8 – 10) are available. Based on the degree of freedom analysis, an additional equation is needed to solve coefficient of hydrocarbons, n_8 . Therefore, additional mass relationship, ratio of mass of hydrocarbons to mass of biomass (R/B) is included in the modified model which considers the hydrocarbons formation. The relationship of temperature and R/B for PKS is determined in Eq. 25.

$$R/B = \frac{T - 647.69}{871.54} \quad (25)$$

4.3 Validation of Model

The models with different temperatures are solved based the constraints in Eqs. 1 – 5, 11 – 20, 22 – 25 via Lingo 13.0 with Global solver at same operating conditions in the experiments. The prediction of major syngas (H_2 , CO , CO_2 , and CH_4) and solid carbon (C) compositions and RMS error are summarised in Table 1. These major syngas and carbon compositions (H_2 , CO , CO_2 , CH_4 and C) are considered in determining the RMS of each biomass. Thus, D term in Eq. 25 is taken as 5 in this work. Table 1 shows the modified model is relatively accurate to predict the composition of syngas and solid carbon. The average RMS of PKS at different temperature is determined as 0.319. It is worth

mentioning that the proposed approach for modelling of gasification is more accurate as compare with previous work (Jarunghammachote and Dutta, 2007) as it has smaller value of RMS errors.

Table 1: Performance data and RMS errors on modified model at different operating temperature

T (K)	1073		1123		1173		1223		1273	
Syngas	mole	RMS	mole	RMS	mole	RMS	mole	RMS	mole	RMS
n_1	8.627		9.999		11.219		12.231		13.159	
n_2	3.331		3.602		3.601		3.281		2.962	
n_3	1.743	0.509	1.610	0.338	1.409	0.335	1.134	0.115	0.924	0.234
n_5	3.475		3.319		3.173		3.069		2.903	
n_7	10.345		9.117		8.215		7.658		7.093	

5. Case Study

Based on the above developed model, the gasifier can be further optimised to achieve various objectives, for example, maximising hydrogen production. Due to limitations of gasifier available in laboratory, additional process constraints are included in the model. In this work, the gasifier is set to operate at temperature (T) is set in the conventional range of 1073 – 1273 K, a pressure (P) of 1 atm, maximum air flowrate (f_i) of 1.1 Nm³/h, and an equivalence ratio (ER) range of 0.23 – 0.27. Based on abovementioned constraints, equations below are included in the model.

$$P = 1 \text{ atm} \quad (26)$$

$$1073 \text{ K} \leq T \leq 1273 \text{ K} \quad (27)$$

$$f_i \leq 1.1 \text{ Nm}^3/\text{h} \quad (28)$$

$$0.23 \leq ER \leq 0.27 \quad (29)$$

Since hydrogen fuel from the biomass waste is the best supersede for fossil fuels, it has a great potential to be used as an energy carrier such as fuel cell that can be applied to power cars and factories and also for home usages in the future (Wan Azlina et al., 2011). Therefore, in order to maximise the hydrogen production in gasifier, the optimisation objective is given in Eq. 30.

$$\text{Maximise } n_1 \quad (30)$$

The equations of 1 – 5, 11 – 20, 22 – 29, were solved with maximising hydrogen production (Eq. 30). Based on the optimised result, maximum of 10.07 mol of H₂ is produced and the optimum operating temperature and ER are determined as 1273 K and 0.27. In addition, the composition of syngas CO, CO₂, CH₄ and solid carbon ash are targeted as 2.73 mol, 1.26 mol, 3.21 mol, and 11.35 mol, respectively. The optimum result is summarised in Table 2.

Table 2: Optimised result prediction

Syngas	Value	Syngas	Value	Syngas	Value
Mole Basis		Volume Basis		Mass Basis	
H ₂ , n_1	13.26 mol	H ₂ , n_1	35.59 vol%	H ₂ Yield	28.48 g/kg biomass
CO, n_2	3.18 mol	CO, n_2	8.55 vol%	Ash, n_7	0.11 kg/kg biomass
CO ₂ , n_3	1.02 mol	CO ₂ , n_3	2.74 vol%		
CH ₄ , n_5	2.82 mol	CH ₄ , n_5	7.57 vol%		
Ash, n_7	6.86 mol				

6. Conclusion

In this work, a modelling of a biomass fluidized bed gasifier based on modified thermodynamic equilibrium model is presented. The proposed model is first validated with the experimental results. Based on the model with correction factor, it can be optimised based on various objective functions to

determine the optimum performance of the gasifier. In the future work, the model is to be further extended for determining optimum operating conditions by taking consideration of ER, bed height, particle size etc.

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