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THERMODYNAMIC ANALYSIS ON HYDROGEN PRODUCTION THROUGH GASIFICATION OF COCONUT SHELL USING A SWIRL FIXED BED GASIFIER

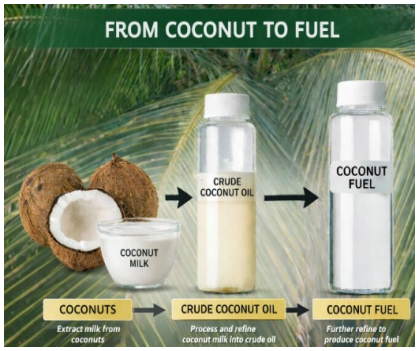
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Graphical abstract



Abstract

The synthesis gas (syngas) produced from the gasification of agricultural waste is an alternative energy to reduce reliance on fossil fuels, which is more sustainable, clean and non-toxic than fossil fuels. In this study, a lab-scale swirl fixed bed gasifier was used to produce hydrogen gases from coconut shells under various operating conditions. A thermodynamic equilibrium model was developed using solver software to predict syngas production, it is simple to use for preliminary comparison and assessment of the gasification process. The results in this study were shown as a comparison between literature models, experimental results, and equilibrium models. This analysis highlights that hydrogen production rises with the moisture content with the highest value of 29.06 vol% at 35% of moisture content at a temperature of 750°C. In temperature evaluation, the hydrogen yield is uncertain according to the temperature. However, the highest temperature obtains 27.98 vol% at 750°C with 25% of moisture content. In short, temperature and moisture content play an important role in determining the synthesis gas produced in gasification. Therefore, based on this study, the best operating condition to enhance hydrogen yields is computationally measured at high moisture content and temperature in the range of 750°C to 850°C.

Keywords: Synthesis gas, Gasification, coconut shell, Thermodynamic equilibrium model, Hydrogen, Moisture content, Temperature

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Abstrak

Gas sintesis (singas) yang dihasilkan daripada penggasan sisa pertanian merupakan tenaga alternatif untuk mengurangkan kebergantungan kepada bahan api fosil, yang mana lebih mampan, bersih dan tidak bertoksik berbanding dengan bahan api fosil. Dalam kajian ini, penggas lapisan tetap pusaran berskala makmal digunakan untuk menghasilkan gas hidrogen daripada tempurung kelapa di bawah pelbagai keadaan operasi. Model keseimbangan termodinamik telah dibangunkan menggunakan perisian penyelesai untuk meramal pengeluaran syngas, ia mudah digunakan untuk perbandingan awal dan penilaian proses penggasan. Keputusan dalam kajian ini ditunjukkan sebagai perbandingan antara model sorotan, keputusan eksperimen, dan model keseimbangan. Analisis ini menyerlahkan bahawa pengeluaran hidrogen meningkat dengan kandungan lembapan dengan nilai tertinggi 29.06 vol% pada 35% kandungan lembapan pada suhu 750°C. Dalam penilaian suhu, hasil hidrogen tidak menentu mengikut suhu. Walau bagaimanapun, suhu tertinggi memperoleh 27.98 vol% pada 750°C dengan 25% kandungan lembapan. Secara ringkasnya, suhu dan kandungan lembapan memainkan peranan penting dalam menentukan gas sintesis yang dihasilkan dalam penggasan. Oleh itu, berdasarkan kajian ini, keadaan operasi terbaik untuk meningkatkan hasil hidrogen diukur secara pengiraan pada kandungan lembapan dan suhu tinggi dalam julat 750°C hingga 850°C.

Kata kunci: Gas sintesis, Penggasan, Tempurung kelapa, Model keseimbangan termodinamik, Hidrogen, Kandungan lembapan, Suhu

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1.0 INTRODUCTION

Animals and plant residues can become renewable material more commonly known as Biomass [1]. Rapid population growth has allowed biomass to be a substitute for fossil fuels. This is driven by the ability of biomass to generate clean energy such as hydrogen energy with carbon dioxide that is environmental-friendly [2]. It is undeniable that fossil fuel has been powering the economy for over a century and currently supplies over 80% of the world's energy [3]. Fossil fuel exists in oil, coal, and natural which are then mainly used to generate electricity and transportation. Unfortunately, continuous fossil fuels consumption leaves disadvantages to the world such as air pollution, the greenhouse gas effect, global warming, and climate change [4], causing many to favour renewable sources.

Biomass does not emit gases that contribute to greenhouse effect and is able to produce energy according to the desired amount [4]. Biomass feedstock can be converted to hydrogen-rich synthesis gas (syngas) through gasification process. Gasification of biomass is one of the processes for renewable energy sources produced by the improvement process of biomass, which is a thermochemical conversion process of a liquid or solid fuel into a highly valuable producer gas by assisted from presence of a gasifying agents such as carbon dioxide, air, oxygen, and steam.

The process supplied low oxygen to complete the combustion of the fuel. Gasification occurs at temperatures between 600°C and 1500°C and yet produces a low to medium energy gas, depending upon the process type and operating conditions [5, 6]. The process called carbonisation refers to the devolatilisation of an organic feedstock to yield gas and char. Syngas can be burned directly, used as fuel for internal combustion engines, or converted to clean diesel fuel through the Fischer-Tropsch process or potentially used in the production of methanol and hydrogen [7, 8]. Due to its environmental friendliness and clean fuel characteristics, syngas is a potential alternative energy source [9, 10, 6].

Syngas (synthesis gas) which is the product of high-temperature steam or oxygen gasification of biomass, consists of a mixture of carbon monoxide (CO) and hydrogen (H_2) [6]. Additionally, the composition of syngas consists of 40% carbon monoxide (CO) as a combustible gas, 25% to 30% of hydrogen (H_2) and 0% to 5% of methane (CH_4), while, the rest are non-combustible gases such as nitrogen (N_2) and 5% to 15% of carbon dioxide (CO_2). However, the compositions depend on the feedstock and the gasification process involved [11, 12]. It has been shown that syngas can be produced from various sources, including biomass, coal, natural gas, or any hydrocarbon feedstock, that reacts with steam or oxygen. Syngas generated from renewable sources is considered as versatile as it can be applied to various uses such as transportation fuel and electricity generation. Moreover, the combination of CO and H_2, can also act as a fuel to produce heat and power or as an intermediary to produce liquid fuel such as diesel fuel, dimethyl ether and methanol [14, 13].

In Malaysia, rapid economic growth is the key factor in increasing energy demand. Malaysia has

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been seen as the diversification of energy sources such as fossil and renewable energy. The renewable energy sources described in Table 1 are widely available in the country. One of the largest sources is biomass. Biomass as renewable energy resources in the world is abundant in the country [14]

Table 1 Renewable Energy Resources in Malaysia [15]

Renewable Energy	Potential (MW)
Biomass	29,000
Biogas	250
Large Hydro	29,000
Mini Hydro (Total Hydro potential is 22,000 MW)	500
Solar PV	6,500
Municipal waste	400

Biomass can be obtained from many sources such as animal manure and municipal waste or agriculture and food processing. However, coconut is deemed as one of the most practical sources of biomass and is available worldwide. Coconut is one of the potential sources of renewable energy which are known available worldwide. According to Rout [16], coconut is a well-known plant grown in more than 90 countries worldwide and the annual world production of coconut is approximately 55 million tonnes. Coconut oil is the main product generated, and possess many applications such as laundry soaps, surface-active agents and hair tonics cosmetics. In Malaysia, coconut as acts as sources of food and economy, especially to the rural households. Approximately 63% of coconut production, oil fronds and shells represent amounts as the biggest waste (about 8% estimations of the potential and current selected biomass utilizations in annual energy productivity in Malaysia) [17]. Wachid *et al.* [18] believed that coconut shell is an underutilised waste as the content of the coconut may be beneficial for humans. Coconut shell has a rigid layer, with a thickness of 3 to 5 mm that contains cellulose, methoxyl, lignin and various mineral. Therefore, coconut shell can be used as a feedstock for gasification process to obtain hydrogen production. Through this process, the raw materials used in the form of solid will be converted into gas. Therefore, in this research, the stoichiometry equation for hydrogen production in gasification of coconut shell will be determined and the effect of temperature and moisture content on the gasification of coconut shell will be analysed using equilibrium model.

2.0 METHODOLOGY

In this study, the stoichiometric equation developed, is a model of stoichiometric thermodynamic equilibrium (STE). The use of STE is simple, but deviations between the model and experimental results may occur as various assumptions were made when formulating this model. The equilibrium from the system response may not be achieved during the experiment. In order to estimate the constant value, modifications are made. Modifications increase the number of predictions, so comparing the predictions obtained through the model with the results obtained through experiments is necessary to determine the accuracy of this model [19]. Table 2 and Table 3 illustrates the proximate analysis and ultimate analysis of coconut shell by Hoque et al. [20], Rupesh et al. 2014 [21] and experiments conducted in Universiti Teknologi Malaysia (UTM) combustion laboratory scale using a swirl fixed bed gasifier.

Table 2 Proximate analysis of coconut shell

Researcher	Moisture Content (%)	Volatile Matter (%)	Fixed Carbon (%)	Ash (%)
Lit. Model 1 [20] (a)	5.36	72.30	21.94	0.4
Lit. Model 2 [21] (b)	8	71	17	4
UTM Lab Experiment (c)	6.86	72.55	15.69	4.9

Table 3 Ultimate analysis of coconut shell

Researcher	C(%)	H_2 (%)	O_2 (%)	N(%)	S(%)	HHV (MJ/kg)
Lit. Model 1 [20] (a)	48.92	6.15	36.85	0.3	0.8	20.58
Lit. Model 2 [21] (b)	45.61	5.61	48.16	0.26	0.34	19.33
UTM Lab Experiment (c)	45.5	6.1	48.16	0.21	0.03	17.49

2.1 MODEL AND DEVELOPMENT

According to Ayub *et al.* [22], there are ten assumptions that have been considered in developing the stochiometric thermodynamic equilibrium model. These assumptions are:

(1) The biomass feedstock consists of hydrogen, carbon, oxygen and nitrogen.
(2) Metal and alkalis content in biomass are neglected
(3) Ash is considered inert
(4) The syngas consists of $H_2, CO, CO_2, CH_4, H_2O$ and N_2.
(5) The negligible amount of tar produced from the downdraft gasifier.

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(6) The feedstock of the biomass and air enter the gasifier at the temperature of 25°C and pressure of gasifier is 101.13 kPa.
(7) The system is assumed as adiabatic and no heat loss from the system.
(8) All reactions inside the gasifier achieved equilibrium.
(9) All gases of the developed system are assumed as ideal gases
(10) N_2 is not included in any chemical reaction.

The typical molecular formula of coconut shell, according to the ultimate and proximate analysis and based on one mol of carbon, is given in Equation (1). The derivation of the equations used to find the unknowns are shown in the following equations.

$$CH_{1.51}O_{0.57} + \omega H_2O + mO_2 + pmN_2 = x_1H_2 + x_2CO + x_3CO_2 + x_4H_2O + x_5CH_4 + pmN_2 \quad (1)$$

Where,

Carbon balance: $1 = x_2 + x_3 + x_5$

Hydrogen balance $2w + 1.51 = 2x_1 + 2x_4 + 4x_5$
$\rightarrow w + 0.755 = x_1 + x_4 + 2x_5$

Oxygen balance $w + 0.57 + 2m = x_2 + 2x_3 + x_4$

The equilibrium constant of methanation reaction.

$$K_{1,CH4} = \frac{x_5}{{x_1}^2} \quad (2)$$

Water gas shift reaction for the equilibrium constant.

$$K_{2\,wgs} = \frac{x_1x_3}{x_2x_4} \quad (3)$$

Moisture content is assumed to be in one mol of biomass and is estimated using Equation (4). The value of w will become constant since the moisture content in the gasification has been determined.

$$MC = \frac{18w}{24 + 18w} \times 100\% \quad (4)$$

Assuming the process of gasification is adiabatic, the heat balance equation is as follows.

$$H^0_{f\ coconut\ shell} + w\left(H^0_{f\ H_2O(l)} + H_{(vap)}\right) + mH^0_{f\ O_2} + 3.76mH^0_{f\ N_2} = x_1H^0_{f\ H_2} + x_2H^0_{f\ CO} + x_3H^0_{f\ CO_2} + x_4H^0_{f\ H_2O\ (vap)} + x_5H^0_{f\ CH_4} + \Delta T\left(x_1C_{P_{H_2}} + x_2C_{P_{CO}} + x_3C_{P_{CO_2}} + x_4C_{P_{H_2O}} + x_5C_{P_{CH_4}} + 3.76mC_{P_{N_2}}\right) \quad (5)$$

At ambient temperature, the values of $H^0_{f\ H_2O(l)}$, $H^0_{f\ N_2}$ and $H^0_{f\ O_2}$ are zero. Thus, equation is simplified become equation 23.

$$H^0_{f\ coconut\ shell} + w\left(H^0_{f\ H_2O(l)} + H_{(vap)}\right) = x_2H^0_{f\ CO} + x_3H^0_{f\ CO_2} + x_4H^0_{f\ H_2O\ (vap)} + x_5H^0_{f\ CH_4} + \Delta T\left(x_1C_{P_{H_2}} + x_2C_{P_{CO}} + x_3C_{P_{CO_2}} + x_4C_{P_{H_2O}} + x_5C_{P_{CH_4}} + 3.76mC_{P_{N_2}}\right) \quad (6)$$

The specific heat of gas and enthalpy change used is shown in Table 4.

Table 4 Specific Heat and Enthalpy change of gas used [10].

Gas	Specific Heat (kJ/kmol K)	Enthalpy Change (kJ/mol)
H_2O	37.36	28594
H_2	29.63	22963.25
CO	31.16	24304
CO_2	48.33	37455.75
N_2	30.75	23831.25
CH_4	56.55	43826.25

The equilibrium constant K in terms of temperature can be written as follows [9].

$$-RTlnK = \Delta G° \quad (7)$$

Note that $\Delta G°$is Gibbs free function of formation and $\Delta H°$ is the heat of formation.

$$\frac{d(\Delta G°/RT)}{dT} = \frac{\Delta H°}{RT^2} \quad (8)$$

Rearranging Equation (9) result in,

$$\frac{\Delta G°}{RT} = -\ln K \quad (9)$$

Substituting equation (10) into equation (11) gives,

$$\frac{d\ln K}{dT} = \frac{\Delta H°}{RT^2} \quad (10)$$

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Therefore,

$$\ln K = \int \frac{\Delta H^{\circ}}{RT^2}_{dT+I} \tag{11}$$

Note that *I* is an integration constant, J is a constant and $\Delta A, \Delta B, \Delta C, \Delta D$ are the coefficient for determined specific heat. The following equation is used to determine the constant J.

(12)

$$\frac{\Delta H^{\circ}}{R} = \frac{J}{R} + (\Delta A)T + \frac{\Delta B}{2}T^2 + \frac{\Delta C}{3}T^3 - \frac{\Delta D}{T}$$

Substituting equation (12) into equation (13),

$$\ln K = \frac{-J}{R} + (\Delta A)\ln T + \frac{\Delta B}{2}T + \frac{\Delta C}{6}T^2 + \frac{\Delta D}{2T^2} + I \tag{13}$$

Replacing equation (10) into equation (12) then multiply with (-RT) results in,

$$\Delta G^{\circ} = J - RT\left((\Delta A)\ln T + \frac{\Delta B}{2}T + \frac{\Delta C}{6}T^2 + \frac{\Delta D}{2T^2} + I\right) \tag{14}$$

Obtaining the specific heat,

$$\Delta A = A_{CH_4} - A_C - 2A_{H_2} \tag{15}$$

$$\Delta A = 1.702 - 1.771 - 2(3.249) = 1.702 - 1.771 - 6.498 = 6.567$$

$$\Delta B = B_{CH_4} - B_C - 2B_{H_2} \tag{16}$$

$$\Delta B = \left(9.081 - 0.771 - 2(0.422)\right) \times 10^{-3} = 7.466 \times 10^{-3}$$

$$\Delta C = C_{CH_4} - C_C - 2C_{H_2} \tag{17}$$

$$\Delta C = \left(-2.164 - 0 - 2(0)\right) \times 10^{-3} = -2.164 \times 10^{-6}$$

$$\Delta D = D_{CH_4} - D_C - 2D_{H_2} \tag{18}$$

$$\Delta D = (0.867 - 0.1666) \times 10^{-5} = 0.701 \times 10^{5}$$

The Gibbs energy formation [9],

$$\Delta H^{\circ}_{298} = (\Delta H^{\circ}_{298})_{CH_4} - (\Delta H^{\circ}_{298})_C - 2(\Delta H^{\circ}_{298})_{H_2} \tag{19}$$

$$\Delta H^{\circ}_{298} = -74{,}520 - 0 - 2(0) = -74{,}520\ J/mol$$

$$\Delta G^{\circ}_{298} = (\Delta G^{\circ}_{298}) - (\Delta G^{\circ}_{298})_C - 2(\Delta G^{\circ}_{298})_{H_2} \tag{20}$$

$$\Delta G^{\circ}_{298} = -50{,}460 - 0 - 2(0) = -50{,}460$$

By substituting all the values into Equation (20) at temperature 298.15°C.

$$\frac{-74520}{R} = \frac{J}{R} + (-6.657)(298.15) + \frac{7.466 \times 10^{-3}}{2}(298.15)^2 + \frac{-2.164 \times 10^{-6}}{3}(298.15)^3 - \frac{0.701 \times 10^{5}}{(298.15)} \tag{21}$$

$$\frac{J}{R} = -7{,}083.18$$
$$J = -58{,}889.6$$

And further calculation in equation (21) to obtain I.

$$-50{,}460 = -58{,}889.6 - (8.314)(298.15)\left((-6.567)\ln(298.15) + \frac{7.466 \times 10^{-3}}{2}(298.15) + \frac{-2.164 \times 10^{-6}}{6}(298.15)^2 + \frac{0.701 \times 10^{5}}{2(298.15)^2} + I\right) \tag{22}$$

$$I = 32.544$$

The general equation for K_1 is

$$\ln K_1 = \frac{70828.48}{T}(-6.567)\ln T + \frac{7.466 \times 10^{-3}}{2}T + \frac{-2.164 \times 10^{-6}}{6}T^2 + \frac{0.701 \times 10^{5}}{2(T)^2} + 32.544 \tag{23}$$

Same procedure is applied to obtain K_2. Therefore, the general equation for K_2 as follows.

$$\ln K_2 = \frac{5872.45}{T} + 1.86\ln T - 2.69 \times 10^{-4}T - \frac{58200}{T^2} - 18 \tag{24}$$

2.2 MATERIAL PREPARATION AND EXPERIMENTAL SET UP

Coconut Shell are stored in room temperature and is shattered into smaller pieces using a hammer. Each sample are then placed inside a grinder to create fine powder. The coconut powder is used for ultimate analysis using an Elementar Vario Micro Cube, Germany device is used by the University Laboratory Management Centre (ULMC) at Universiti Teknologi Malaysia (UTM) using an ISO 16948:2015 standard.

The proximate analysis utilises several standards. ISO 18134-2: 2015 is used to analyse the moisture content of the sample. For volatile matter, the

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standard used is ISO 18123: 2015 and ISO 18122: 2015 is used for the ash content.

While the proximate analysis is to determine moisture content and ash with a controlled temperature of 107±3°C for 1 hour. Once the hour finishes, the samples are cooled until it reaches room temperature. Once it reaches room temperature, the sample is weighed. The moisture content is determined by using the following formula.

$$Moisture\ Content\ (\%) = \frac{a-b}{a} \times 100\% \quad (25)$$

Where a = initial mass of sample (g)
b = final mass of sample after cooling (g)

The samples are then heated again at 950°C for 7 minutes. The samples then undergo cooling and weighed. The difference in mass is noted as the volatile matter content. Lastly, the final heating at temperature of 750°C for 8 hours for the samples. The same process is carried out and cooled before weighed. The formula used to determine the ash content of the sample is,

$$Ash\ Content\ (\%) = \frac{d}{c} \times 100\% \quad (26)$$

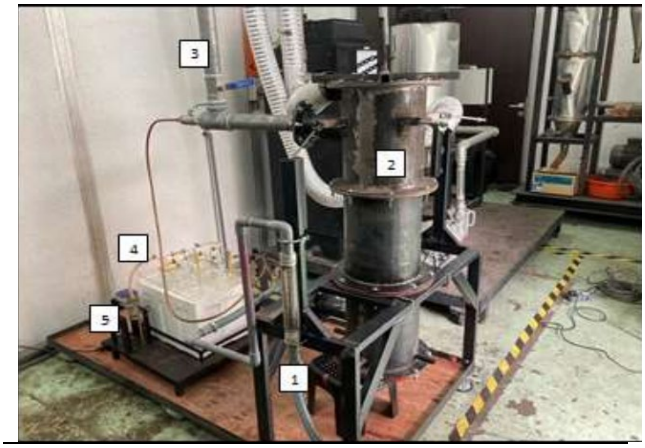
Where d = initial mass of sample (g)
c = final mass of sample after cooling (g)

The fixed carbon content then calculated using a difference method, which subtracts the summation of moisture content, volatile matter, ash content and fixed carbon from 100%.

2.3 GASIFICATION PROCEDURE

For this gasification procedure, the drying process is considered complete once the material reached approximately 150°C or a moisture content of 18± 2%. The fixed bed gasifier used for this experiment is laboratory-scaled, meaning that it is mobile (installed on movable platform) and operating at atmospheric pressure. Air acts as a gasifying agent and adjusted to a flow rate of 20 m^3/hr. The cylindrical – shaped has an inside diameter of 40cm, thickness of 6 cm and 1 m in length, is made of mild steel which can withstand temperature up to 1100°C. The coconut shell is poured into the gasifier from the top of the reactor chamber. Approximately 5 kg of feedstock is used in one combustion cycle. Air enters the furnace in co-current flow with the feedstock along with the carrier gas. The cyclone will remove ash and particles from the gas and transfer them into the ash collector, connected to the bottom of the cyclone. The gas is collected once the flame of gas is produced. Syngas is then directed into the tar sampling train, before finally reaching the Tedlar bags where syngas is stored to be analysed. Based on Figure 1, there are five main parts involve in the installation of the gasifier. Figure 2 describes the schematic of the swirl fixed bed gasifier used for this study.

The tar sampling train is illustrated in Figure 3. The first four impinger bottles are each filled with 100 ml of isopropanol, whereas bottles 5 and 6 are filled with silica gel. Impinger bottles filled with Isopropanol must be kept in an ice bath and its temperature - maintained at -15°C.



No.	Name of parts	No.	Name of parts
1	Air flow meter	2	Combustion chamber
3	Exhaust	4	Tar sampling system
5	Gas collector		

Figure 1 Swirl fixed bed gasifier installation

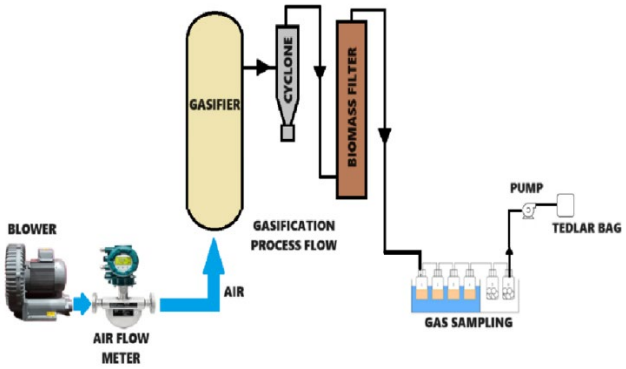


Figure 2 Schematic of swirl fixed bed gasifier

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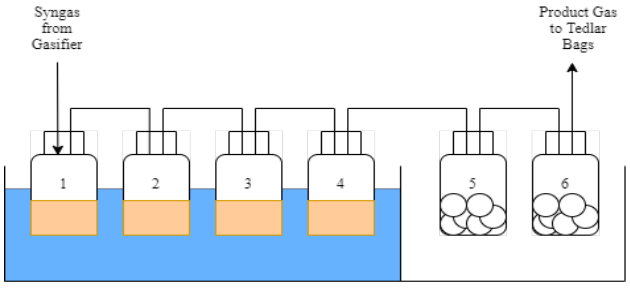


Figure 3 Tar sampling system. Bottles 1 – 4 are filled with 150 ml of isopropanol whilst bottles 5 and 6 are filled with silica gel

3.0 RESULTS AND DISCUSSION

3.1 MODEL VERIFICATION

Table 5 illustrates differences in the synthesis gas produced through simulation, STE model and from experiment. The absolute error is calculated to check the validation of the equilibrium model. By referring to the results in Table 5, all synthesis gas composition has minor absolute error when comparing to the literature model and experimental (Figure 4). This due to the different values used for the specific heat of the gas and the enthalpy change in the analysis. Research conducted by Korones and Lykidou [23] is used as the main reference for this study to determine the specific heat of the gas and enthalpy change for each of the gases. From the analysis, it is observed that CO_2 and H_2 were over-predicted while CH_4 and CO were underpredicted by the equilibrium model compared to the experimental value. While comparison between the equilibrium model and the literature models showed that all values are below expectations.

According to Figure 4, the composition of hydrogen in syngas increases continuously with the moisture content. A similar trend is also observed for carbon dioxide. On the other hand, the percentage of carbon monoxide reduces for the same variation of moisture content. The same is also observed for the composition of the methane. In the absolute error section (a-d), it was found that CO_2 obtained the highest value at 9.37% compared to H_2 and CO, while CH_4 produced the lowest absolute error value at 0.53%. Higher error found in CO_2 is caused by the exothermic water gas shift reaction. While the lowest error found in CH_4 composition is due to the combined effect of the transition of the endothermic steam methane reforming reaction and the exothermic methane reaction, which favours product side and the reaction side, respectively. The error found in H_2 gas and CO composition is 7.13% and 1.43% respectively. Error found in H_2 composition is because of the exothermic water gas shift reaction, where higher temperature results in the reversal of the reaction. In addition, CO concentration increases with temperature and the rate of increase is more at lower temperature ranges. This is due to the combined effect of endothermic char gasification, water gas and methane reformation and reversal water gas shift reaction [23, 21].

The absolute error for section (c-d) illustrates difference between the equilibrium model and the laboratory experiment. The absolute error for H_2 is 13.58%. This value is the highest value amongst all the other H_2 gas absolute errors. The CO_2 absolute error is 6.57% whilst the value of CO and CH_4 are 1.37% and 1.85% respectively. Slight variation in H_2 concentration was successfully predicted by the model, except for the experiment carried out [24]. This could be related to the variation in moisture content that influences H_2 concentration in the syngas [25].

As expected, the obtained results are evidence of major limitation found in both model lies in the thermodynamic equilibrium assumption. In fact, results showed that syngas composition is better reproduced for biomass that are low in ash content and consequently a relatively high heating value. As the gasification bed temperature increases, generally the deviation between numerical results and experimental results also increased. Otherwise, using of the equilibrium model results in a closer prediction to the experimental values, minimising the error between simulated and experimental data. This is especially true for CH_4 concentration, which being very low in values, which makes them difficult to model [25].

3.2 EFFECT OF MOISTURE CONTENT IN SYNTHESIS GAS PRODUCTION

The same coding is reapplied to identify the relationship between the moisture content and the synthesis gas composition. The moisture content investigated ranges between 10% to 35%. Using the same molecular feedstock biomass ($CH_{1.51}O_{0.57}$) at a constant temperature of 750°C. Syngas composition that are highlighted here are hydrogen gas, carbon dioxide, carbon monoxide, methane, and nitrogen gas.

The influence of coconut shell's moisture content on H_2 production can be seen clearly in Figure 5. An increase in moisture seemed to generally increase H_2 gas production. The highest volume of H_2 gas obtained in this investigation is 29.06 vol% at moisture content 35% meanwhile the lowest hydrogen gas produced is 25.75 vol% at 10% moisture content goes to CO_2, the production of this gas increases linearly with the moisture content. Among others synthesis gas, CO_2 has a steeper gradient compared to H_2 and CO_2 which means minute moisture increment leads to significant CO_2 production.

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Table 5 Comparison between literature model, experimental and simulated equilibrium model

Synthesis gas component	Lit. Model 1 [20] (a)	Lit. Model 2 [21] (b)	UTM Lab Exp. (c)	Equilibrium Model (d)	Absolute Error (a-d)	Absolute Error (b-d)	Absolute Error (c-d)
Hydrogen (H_2) %	20.85	21.22	14.4	27.98	7.13	6.76	13.58
Carbon Monoxide (CO) %	25	20.44	22.2	23.57	1.43	3.13	1.37
Carbon Dioxide (CO_2)%	8.2	14.48	11	17.57	9.37	3.09	6.57
Methane (CH_4) %	1.12	1.29	3.5	1.65	0.53	0.36	1.85

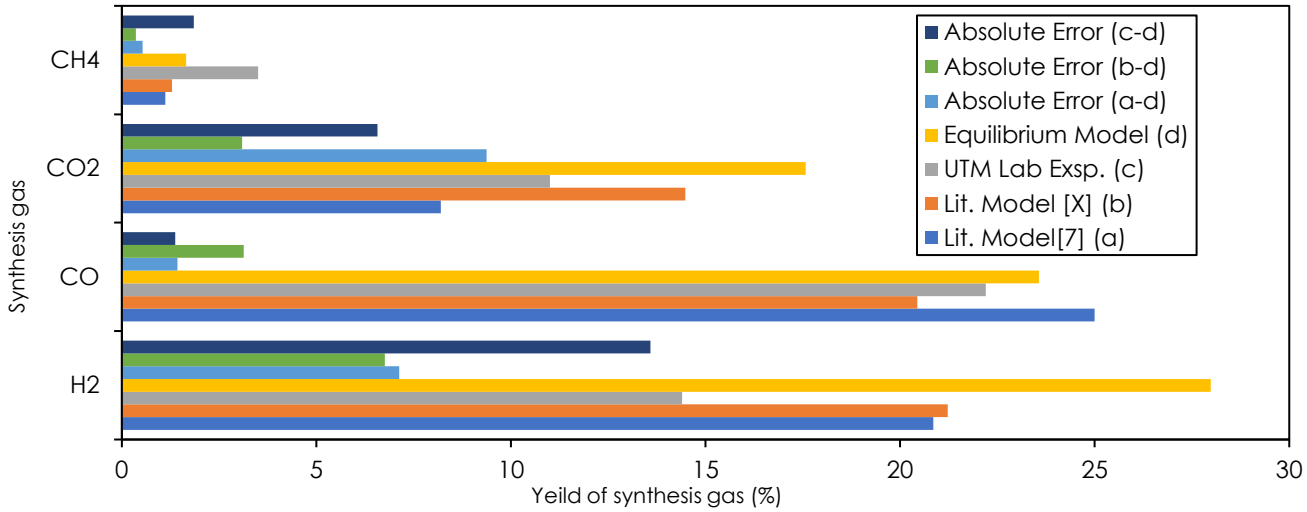


Figure 4 Comparison of literature models, lab experiment and developed model with absolute errors with temperature between 650°C to 1050°C

From the analysis, the maximum and minimum of CO_2 produced are 20.54 vol% at 35% moisture and 13.04 vol% at 10% moisture respectively. On the other hand, methane production may not be influenced by moisture, as minute variation (less than 1 %) were observed with each moisture increment. In addition, N_2 gas production was also analysed in simulation, and small changes of N_2 yield were observed with increasing moisture content. Generally, Figure 5 suggested that the relationship between nitrogen yield is inversely proportional to moisture content.

The advantage of raising the moisture content is reduced carbon monoxide production. This is shown at 10% moisture, where the carbon monoxide yield is 19.24 vol%. On the other hand, when at 35% moisture, the carbon monoxide is 19.24 vol%. Therefore, it can be concluded that higher moisture content results in better syngas composition. This is caused by the reduction in CO content, as high CO presence can damage certain brain structure (basal ganglia and cerebral cortex) and can lead to death [26].

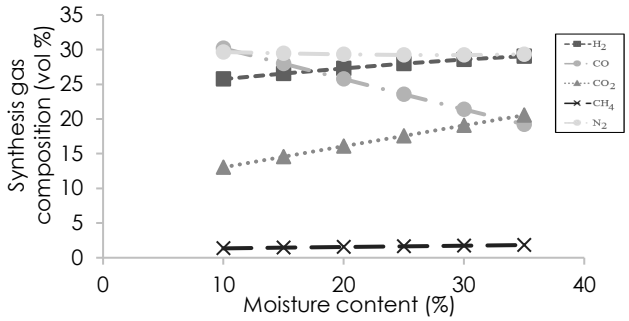


Figure 5 The effect of moisture content on gas composition at temperature 750°C

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3.3 EFFECT TEMPERATURE IN SYNTHESIS GAS PRODUCTION

Figure 6 shows the relationship between temperature variation and syngas yield. The temperature in this investigation ranges from 650°C to 1050°C. Figure 6 displays the trend in synthesis gas generation at various temperature. Increased temperature did not yield a definitive trend in H_2 gas production. The highest H_2 yield in this study is 27.98vol% at temperature 750°C. On the other hand, the CO yield rises gradually as temperature rises. The maximum CO obtained in equilibrium simulation is 29.67 vol% at 1050°C and lowest CO detected at temperature 650°C where 19.77 vol% of CO accumulated. Higher swirl fixed bed temperature will enhance the endothermic reaction that happens in reactions in Equatioan (27) to (29) which lead to increased H_2 and CO production [28]. However, it is noted that further increment of temperature could not improve the H_2 yield. Therefore, the recommended gasification temperature range for high H_2 yield should be between 750°C to 850°C.

The CO_2 yield reduces with temperature increment, starting from 20.74 vol% at 650°C until 13.16 vol% at 1050°C. Observation thus suggests that temperature plays an important role in lessening the CO_2 yields. Like CH_4, the volume percent of methane reduces at the higher temperature. This is because methane formation is limited by an exothermic reaction occurring during gasification stage, as shown in reaction equation (30) [27]. This is shown by the CH_4 yield at 1050°C which is 0.125 vol%. Conversely, N_2 production increases at higher temperature.

$$C + H_2O \rightarrow CO + H_2 \ldots . \Delta H = +118.628\ \text{kJ/mol} \quad (27)$$

$$C + 2H_2O \rightarrow CO_2 + 2H_2 \ldots . \Delta H = +75.114\ \text{kJ/mol} \quad (28)$$

$$C + CO_2 \rightarrow 2CO \ldots . \Delta H = +162.142\ \text{kJ/mol} \quad (29)$$

$$CH_4 + 2H_2 \rightarrow CH_4 \ldots . . \Delta H = -75.24\ \text{kJ/mol} \quad (30)$$

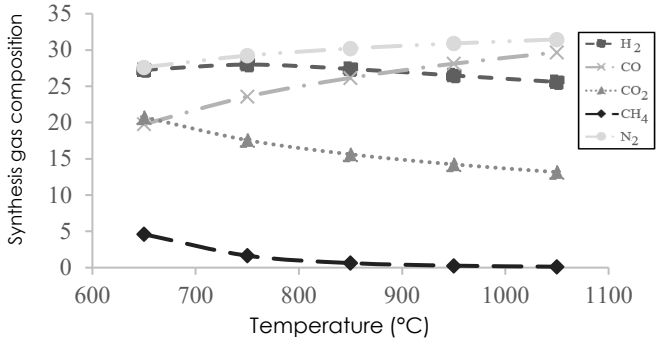


Figure 6 The Effect of Temperature on Synthesis Gas Composition

4.0 CONCLUSION

The objective of this research is achieved, as the equilibrium model managed to predict the performances of synthesis gas at temperatures between 650°C and 1050°C and constant moisture content and various moisture content (10% to 35%) at constant temperature. The result obtained from the simulation equilibrium model was close to the outcome from previous researcher and laboratory experiment with its corresponding error calculated. The observed trends in the two conditions set are as follows:

(1) The hydrogen, carbon dioxide and methane in produced gas increases with the increasing moisture content at constant temperature (750°C).
(2) The carbon monoxide and nitrogen gas decreases with increasing moisture content at constant temperature (750°C).
(3) Temperature increment promotes carbon monoxide and nitrogen gas production at constant moisture (25%) moisture.
(4) The carbon dioxide and methane yield reduce with increasing temperature at constant moisture (25%).
(5) Hydrogen production may not be significantly influenced by increasing temperature at constant temperature (25%).

The highest hydrogen production in this study is 29.06 vol% at optimal operation conditions which are: 35% moisture and a temperature of 750°C. In general, the equilibrium model could predict the composition of synthesis gas in coconut shell gasification with different operating conditions such as varied moisture content and temperature. Furthermore, the result shows that both parameters play a role in syngas production. In brief, the equilibrium model created can be used widely to any biomass feedstock by setting the molecular formula of biomass feedstock to the 1 mol of carbon, temperature, and moisture content.

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Conflicts of Interest

The authors declare that there is no conflict of interest regarding the publication of this paper.

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Data availability

The data supporting the findings of this study are available from the corresponding author upon reasonable request.

Ethics declaration

Formal ethical approval was not obtained for this study. However, the authors confirm that the research was conducted in accordance with established ethical principles and good research practices, with due consideration given to participant rights, informed consent, confidentiality, and responsible data handling.

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