PAPER • **OPEN ACCESS**

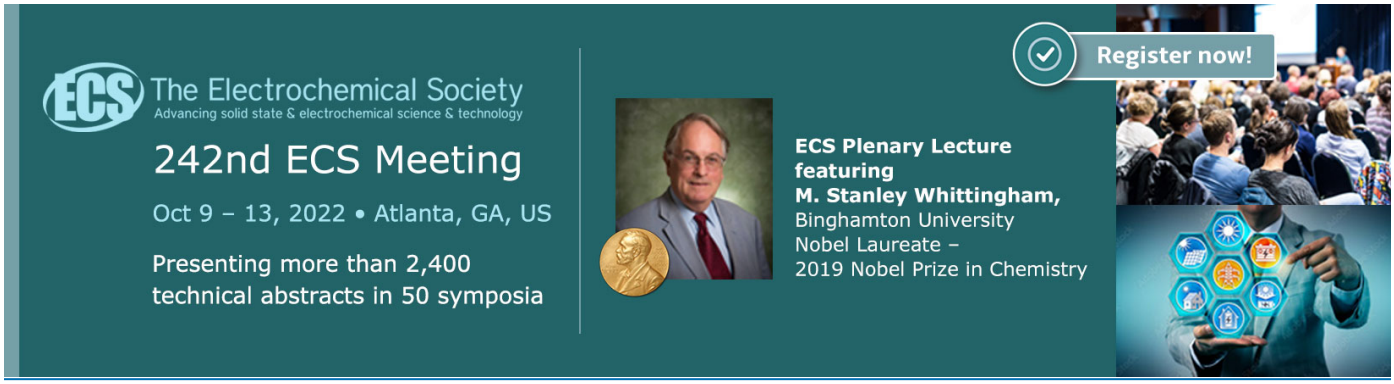
Syngas software for biomass gasification process

To cite this article: S Saleh and N A F A Samad 2019 *IOP Conf. Ser.: Mater. Sci. Eng.* **702** 012007

View the article online for updates and enhancements.

You may also like

- Performance modelling and validation on co-gasification of coal and sawdust pellet in research-scale downdraft reactor
F Z Mansur, C K M Faizal, A F A Samad et al.
- Strategy for Carbon Gasification from Porous Ni-YSZ Anodes of Industrial-Sized ASC-SOFCs and Effects of Carbon Growth
Vanja Suboti, Christoph Schluckner, Bernhard Stöckl et al.
- Gasification of empty fruit bunch with carbon dioxide in an entrained flow gasifier for syngas production
N F H Rahmat and R A Rasid



This content was downloaded from IP address 103.53.32.15 on 21/09/2022 at 03:34

IOP Conf. Series: Materials Science and Engineering **702** (2019) 012007 doi:10.1088/1757-899X/702/1/012007

Syngas software for biomass gasification process

S Saleh and N A F A Samad*

Faculty of Chemical and Process Engineering Technology, College of Engineering Technology, Universiti Malaysia Pahang, 26300 Gambang, Pahang, Malaysia

*E-mail: asmafazli@ump.edu.my

Abstract. In this work, the thermodynamic equilibrium model has been developed in Excel software for evaluating gasification process. The software is called as Syngas software is applicable to study the effects of gasification temperature either using air or steam as gasifying agents for a wide range of biomass. The application of Syngas software has been highlighted through gasification of EFB using air as gasifying agents. The effects of gasification temperature between 650°C and 900°C has been conducted. The highest amount of hydrogen gas and carbon monoxide gas produced are 29.4 mol% and 44.1 mol% respectively at gasification temperature of 900°C. Meanwhile around 19.5 mol% of carbon dioxide gas and 5.8 mol% of methane gas have been generated at similar gasification temperature. The thermodynamic equilibrium model developed in the Syngas software has been validated against experimental data where root mean square errors (RMSEs) lesser than 1 is obtained indicating a reliable of the developed Syngas software.

1. Introduction

Recently waste to energy (WtE) is becoming one of the innovative technologies for producing sustainable energy with minimum damage to the ecosystems. Through WtE, the waste produced from household, industries and various other agricultural related activities is transformed into a fuel source or in the form of electricity and/or heat [1-2]. One of the attractive WtE conversion technology is biomass gasification. Biomass gasification process is a widely applied technology for converting solid biomass into synthesis gas. The main components of synthesis gas are hydrogen, carbon monoxide, carbon dioxide and methane [1]. The generated synthesis gas is useful for production of heat, power and gaseous fuel. The synthesis gas can also be used to produce methanol, dimethyl ether (DME) and methyl tert-butyl ether (MTBE) for liquid fuel in transportation [1,3].

Thus extensive works either based on experimental or simulation have been performed by numerous researchers in investigating and studying the gasification using various types of biomass. In terms of experimental works, the effects of gasification temperature has been performed on Eucalyptus wood chips [4]. Effect of temperature on gasification using different types of biomass (switchgrass, hardwood, softwood, fiber, cardboard and chicken manure) has been investigated [5]. The influences of temperature and operation time for oil palm frond (OPF) gasification process have been investigated where optimum synthesis gas can be produced at temperature range between 700 and 900°C [6]. In addition to experimental works, the gasification performance can also be studied using simulation models. Through simulation, the effects of various operating conditions on the gasification performance can be evaluated without relying on experimental setup. The model for gasification process can be developed based on kinetic rate models and a thermodynamic equilibrium model. Usually the thermodynamic equilibrium model is preferable due to its simplicity, is easy to develop and the maximum achievable yield under equilibrium conditions can be predicted [7]. Accordingly, a thermodynamic model of a fixed bed gasifier

Content from this work may be used under the terms of the Creative Commons Attribution 3.0 licence. Any further distribution of this work must maintain attribution to the author(s) and the title of the work, journal citation and DOI.
Published under licence by IOP Publishing Ltd

in Cycle-Tempo software has been developed for studying the gasification process [8] and an equilibrium model based on Gibbs free energy minimization has been used in Aspen Plus software to predict the performance of oil palm frond and empty fruit bunch gasification processes [9-10]. In addition the equilibrium model has been developed in order to study thermochemical gasification for agricultural residues [11-12].

Although many experimental and simulation works have been done to study gasification process, but there are some limitations on those approaches. Firstly, the suitability of biomass to be used as a feedstock for gasification. This is depending on its properties such as ultimate analysis and proximate analysis. For example, high moisture content and low fixed carbon of biomass tends to produce low synthesis gas yield [1,9]. Secondly, the optimal operating condition for producing maximum hydrogen gas is different for each biomass. This ultimately consumes a lot of experimental works for finding an optimal condition for biomass to be studied as well as involving trial and error for finding the best biomass to be used as feedstock for gasification process. Based on our literature review, there are most of the model available in literature are applicable for problem specific case study and there is no specific biomass database for studying a wide range of biomass as feedstock for gasification process. Therefore, the objective of this work is to develop a software called as Syngas Software for studying biomass gasification process which is based on thermodynamic equilibrium model. Through this software, it is possible to investigate the synthesis gas production using air or steam. In addition, a database contains around 250 biomass has been developed and integrated with the software in order to applicable for wide range of biomass selection. This in turn helps for evaluating the suitability of biomass as feedstock before it can be implemented in the experimental work.

2. Thermodynamic Equilibrium Model-based Framework for Biomass Gasification Process

In our previous work, the framework for thermodynamic equilibrium model-based has been developed as shown in figure 1 [13].

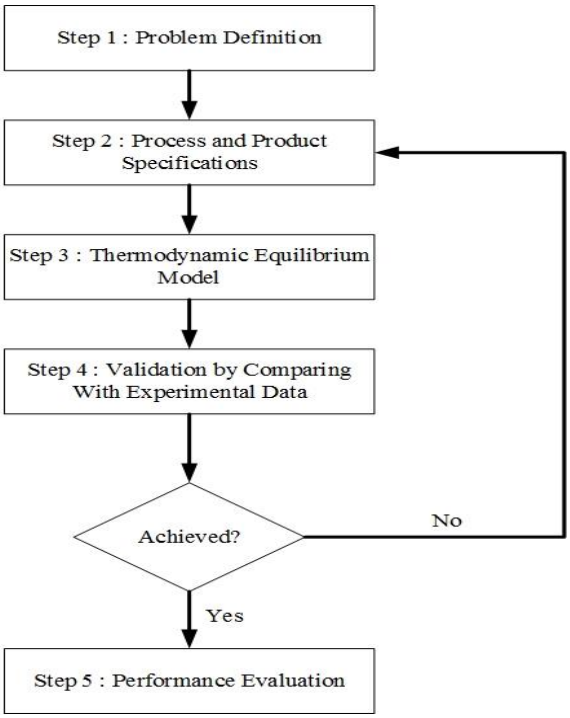


Figure 1. Biomass gasification framework using thermodynamic equilibrium method adopted from [13]

The starting point of this framework is problem definition in terms of objective specification. The example of objectives could be to evaluate gasification performance, to investigate the effects of temperature on synthesis gas production or to compare gasification performance using either air or steam. Based on specified objective, the process and product specifications are performed in step 2. For

process specification, the option to select gasifying agents either air or steam is included. In addition the biomass that needs to be investigated will be selected. Here the user is able to select biomass from the developed database as shown in table 1. In the case of biomass data is not available in our database, the ultimate and proximate analysis need to be provided since these properties are essential for thermodynamic equilibrium model. In terms of product specification, the user able to select the components of synthesis gas such as hydrogen gas or all synthesis gas components.

Table 1. Example of biomass properties in database

No.	Type of Biomass	C	H	O	N	S	References
1	Bamboo	40.64	5.64	44.09	0.52	0.03	[1]
2	Empty Fruit Bunch	43.53	7.20	47.09	1.73	0.46	[9]
3	Oil Palm Frond	43.94	6.94	44.88	3.52	0.72	[14]
4	Palm Kernel Shell	49.91	6.94	38.20	3.52	0.72	[15]
5	Pomace	51.31	6.40	35.01	2.00	0.26	[8]
6	Rice Husk	38.43	2.97	36.36	0.49	0.07	[12]
7	Wood Chips	45.69	4.65	50.32	0	0	[4]
8	Wood Pellet	43.52	7.00	43.53	0.23	0.08	[5]

Step 3 involves the calculation of synthesis gas using thermodynamic equilibrium model. Table 2 shows the thermodynamic equilibrium model based on the selected gasifying agents. The steps needed for applying thermodynamic equilibrium model is shown below:

a) Calculate value of w using equation (1)

$$w = \frac{24MC}{18(1-MC)} \tag{1}$$

b) Determine values of ΔA, ΔB, ΔC and ΔD using information of heat capacities.
c) Calculate values of $\Delta G°$ and $\Delta H°$ at reference temperature.
d) Obtain coefficients of J and I simultaneously using information from a) and b).
e) Calculate equilibrium constants k_1 and k_2.
f) Based on e), the stoichiometries are obtained by using Newton Raphson method.
g) Based on values of stoichiometries, the synthesis gas produced can be calculated using mole balance.

The information for heat capacities, heat of formation and Gibbs of formation at reference temperature can be obtained from [16]. The validation is then performed in step 4 in order to compare the values of synthesis gas obtained from thermodynamic equilibrium model with literature data. The error between the synthesis gas from the experimental work and the thermodynamic equilibrium model is calculated using root mean square error (RMSE) as shown in equation (2).

$$\text{RMSE} = \sqrt{\frac{\sum (X_{\text{exp}} - X_{pred})^2}{N}} \tag{2}$$

Where X_{exp} and X_{pred} are the experimental data and predicted data of synthesis gas respectively and N is the number of data used. If the RMSE obtained is lesser than 1 then the model is classified as reliable indicating the predicted synthesis gas is in good agreement with literature data [12]. Otherwise the user needs to specify process and product again in step 2 in order to reduce the RMSE. Lastly the performance of gasifier is evaluated based on two factors which are synthesis gas produced at different

temperature and different moisture content. Based on these two factors, the best operating conditions can be obtained for improvement and validation of gasification process.

Table 2. General gasification process using thermodynamic equilibrium approach [13]

Gasifying Agent: Air	Gasifying Agent: Steam
$CH_aO_b + wH_2O + mO_2 + 3.76mN_2 = x_1H_2 + x_2CO$ $+x_3CO_2 + x_4H_2O + x_5CH_4 + 3.76mN_2$	$CH_aO_b + wH_2O + mH_2O = x_1H_2 + x_2CO + x_3CO_2$ $+x_4H_2O + x_5CH_4$
Carbon balance: $x_2 + x_3 + x_5 - 1 = 0$	Carbon balance: $x_2 + x_3 + x_5 - 1 = 0$
Hydrogen balance: $2x_1 + 2x_4 + 4x_5 - a - 2w = 0$	Hydrogen balance: $2x_1 + 2x_4 + 4x_5 - a - 2w - 2m = 0$
Oxygen balance: $x_2 + 2x_3 + x_4 - w - 2m - b = 0$	Oxygen balance: $x_2 + 2x_3 + x_4 - w - m - b = 0$

Equilibrium constant:

$$k_1 = \frac{x_5}{(x_1)^2}$$

Equilibrium constant:

$$k_2 = \frac{x_1 x_3}{x_2 x_4}$$

$$\ln k = -\frac{J}{RT} + \Delta A \ln T + \frac{\Delta B.T}{2} + \frac{\Delta C.T^2}{6} + \frac{\Delta D}{2T^2} + I$$

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

$$\Delta G^\circ = J - RT\left[\Delta A.\ln T + \frac{\Delta B.T}{2} + \frac{\Delta C.T^2}{6} - \frac{\Delta D}{2T^2} + I\right]$$

Data on heat capacity:

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

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

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

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

3. Application of Syngas Software

In this work, the gasification process based on thermodynamic equilibrium has been constructed in Excel software which is called as Syngas software. The selection of Excel software is due to its simplicity and accessible. All of the mathematical equations as shown in table 2 has been setup in Excel sheet for ease of the solution. In this section the applicability of the Syngas software is highlighted through the gasification of empty fruit bunch (EFB).

3.1. Problem Definition (Step 1)

The objective of this work is to validate the performance of gasification process as shown in figure 2.

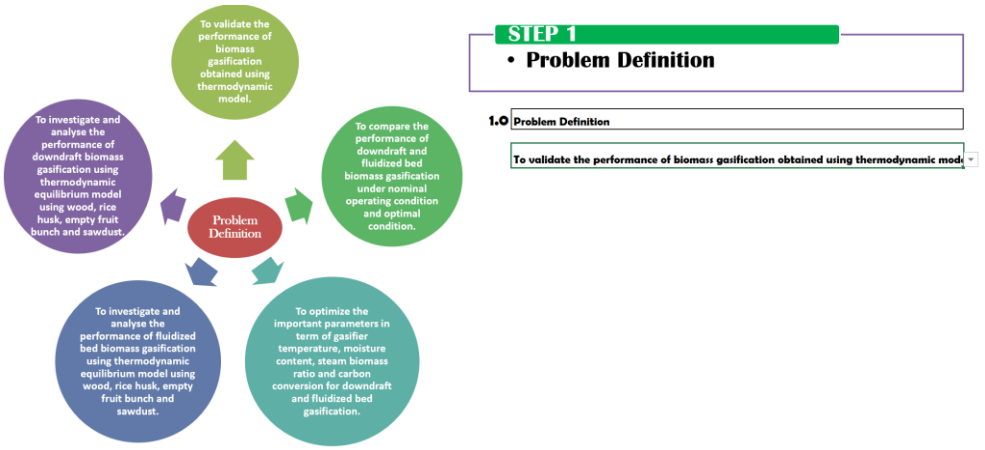


Figure 2. Problem definition (Step 1).

3.2. Process and Product Specifications (Step 2)

In terms of process specification, the gasifying agent selected is air and type of biomass to be studied is empty fruit bunch (EFB) as shown in figure 3. Meanwhile the main product for this work is the amounts of synthesis gas produced. The main variables to be studied for operating condition is gasification temperature.

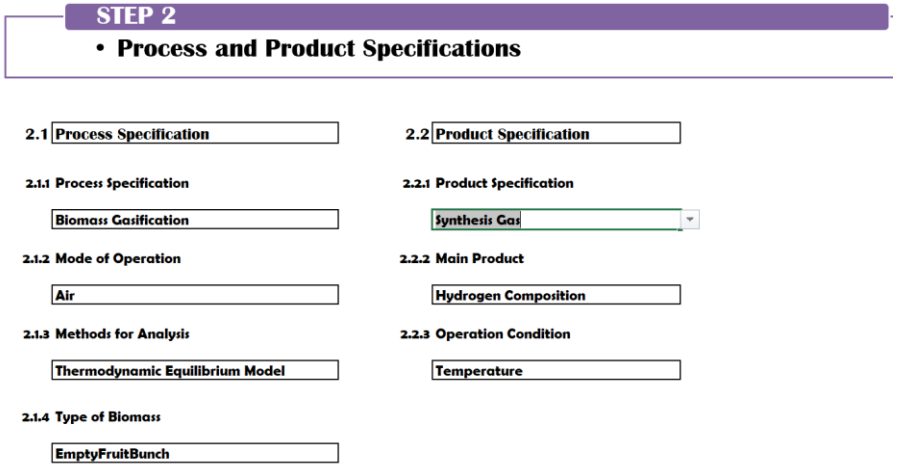


Figure 3. Process and product specifications (Step 2).

3.3. Thermodynamic Equilibrium Model (Step 3)

Based on selection in step 2, the chemical formula for EFB is then extracted from database as shown in figure 4. Notes that the elements of S and N are not considered in this work since both amounts are relatively small and thus neglected. Here the user needs to specify the gasification temperature in the range from 600-1000°C. In addition the moisture content used for this case study is 0.2. Based on this specifications, the model is then performed as shown in figure 5 where the values of ΔA, ΔB, ΔC and ΔD are calculated based on heat capacities for each chemical components. Then Gibbs of formation ($\Delta G°$) and heat of formation ($\Delta H°$) at 25°C are calculated. These values are then used for determining variables *J* and *I* which subsequently used for calculating equilibrium constants k_1 and k_2 as shown in figures 5 and 6 respectively. Based values of equilibrium constants, the coefficients of x_1 (hydrogen), x_2 (carbon monoxide) and x_3 (carbon dioxide) are obtained by using Newton Raphson method as shown in figure 7. Meanwhile the remaining coefficients of x_4 (water) and x_5 (methane) are then obtained by solving the carbon, hydrogen and oxygen balances as shown in figure 8. Lastly the composition of synthesis gas produced can be calculated using mole balance.

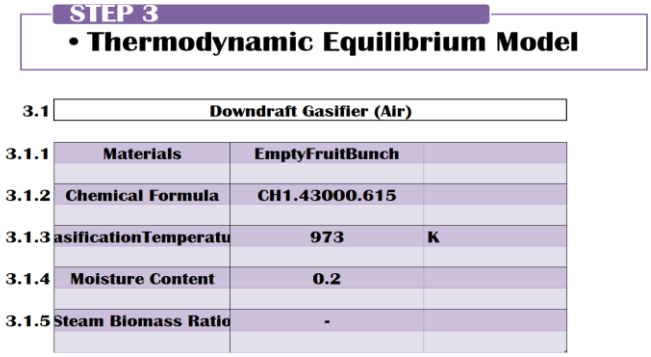


Figure 4. Thermodynamic equilibrium model (Step 3).

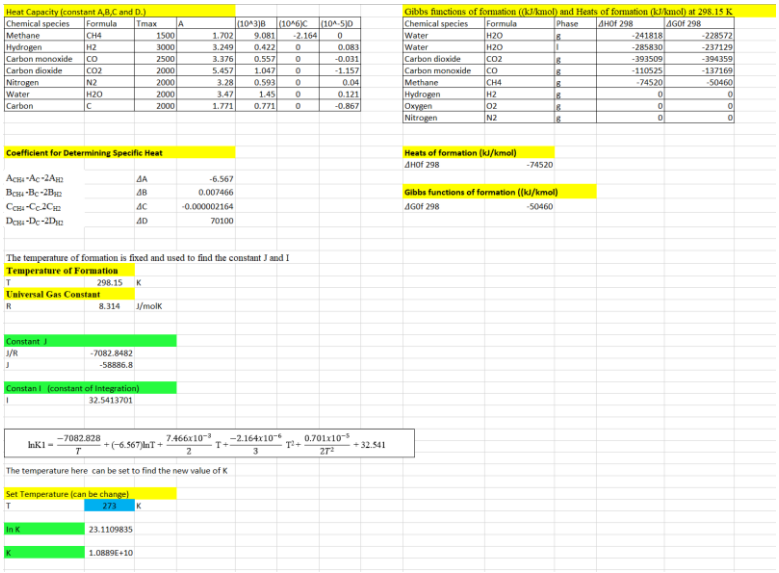


Figure 5. Calculation of equilibrium constant, k_1

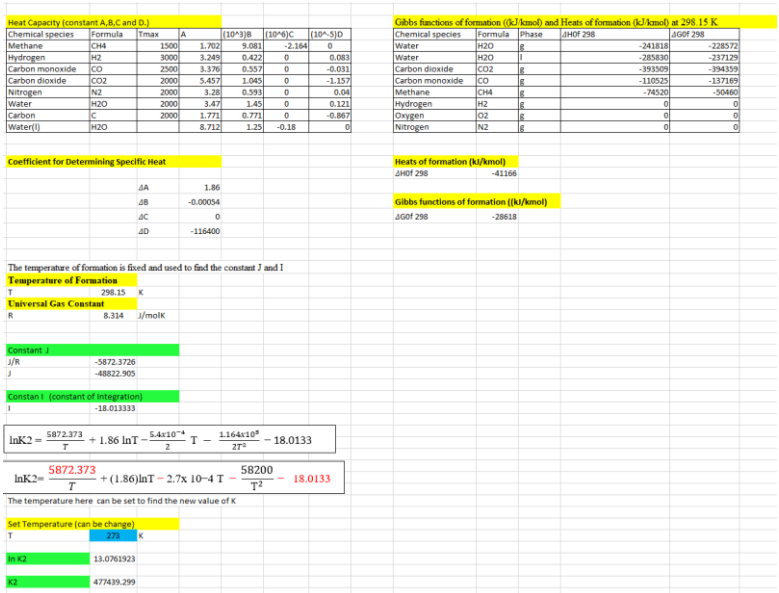
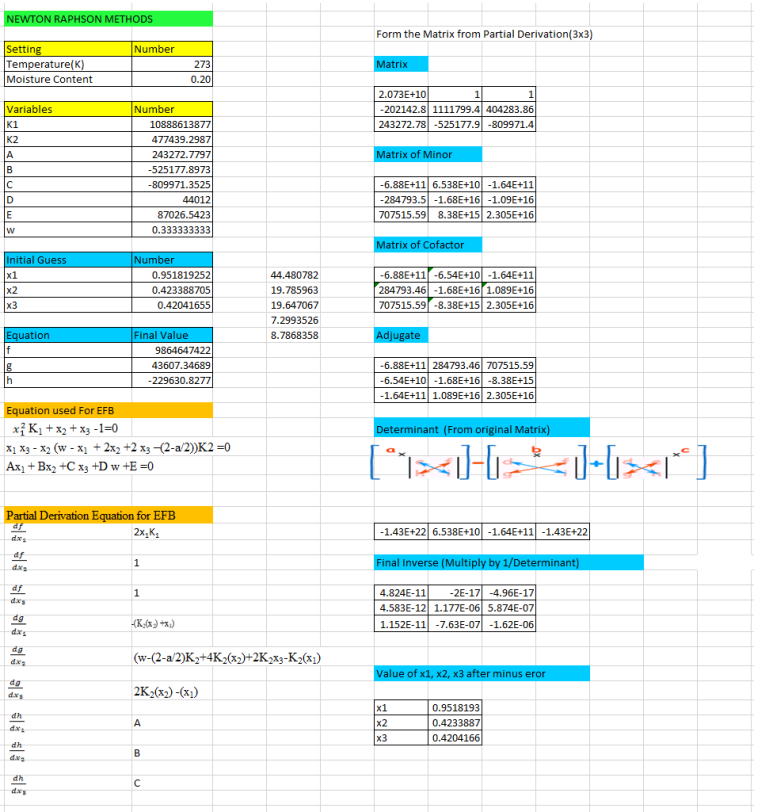


Figure 6. Calculation of equilibrium constant, k_2



NEWTON RAPHSON METHODS

Setting	Number
Temperature(K)	273
Moisture Content	0.20

Variables	Number
K1	10888613877
K2	477439.2987
A	243272.7797
B	-525177.8973
C	-809971.3525
D	44012
E	87026.5423
w	0.333333333

Initial Guess	Number		
x1	0.951819252	44.480782	
x2	0.423388705	19.785963	
x3	0.42041655	19.647067	
		7.2993526	

Equation	Final Value	
f	9864647422	
g	43607.34689	
h	-229630.8277	

Equation used For EFB

$x_1^2 K_1 + x_2 + x_3 - 1 = 0$

$x_1 x_3 - x_2 (w - x_1 + 2x_2 + 2 x_3 - (2-a/2))K2 = 0$

$Ax_1 + Bx_2 + C x_3 + D w + E = 0$

Partial Derivation Equation for EFB

$\frac{df}{dx_1}$	$2x_1K_1$
$\frac{df}{dx_2}$	1
$\frac{df}{dx_3}$	1
$\frac{dg}{dx_1}$	$-(K_2(x_2)+x_3)$
$\frac{dg}{dx_2}$	$(w-(2-a/2)K_2+4K_2(x_2)+2K_2x_3-K_2(x_1)$
$\frac{dg}{dx_3}$	$2K_2(x_2)-(x_1)$
$\frac{dh}{dx_1}$	A
$\frac{dh}{dx_2}$	B
$\frac{dh}{dx_3}$	C

Form the Matrix from Partial Derivation(3x3)

Matrix

2.073E+10	1	1
-202142.8	1111799.4	404283.86
243272.78	-525177.9	-809971.4

Matrix of Minor

-6.88E+11	6.538E+10	-1.64E+11
-284793.5	-1.68E+16	-1.09E+16
707515.59	8.38E+15	2.305E+16

Matrix of Cofactor

-6.88E+11	-6.54E+10	-1.64E+11
284793.46	-1.68E+16	1.089E+16
707515.59	-8.38E+15	2.305E+16

Adjugate

-6.88E+11	284793.46	707515.59
-6.54E+10	-1.68E+16	-8.38E+15
-1.64E+11	1.089E+16	2.305E+16

Determinant (From original Matrix)

-1.43E+22	6.538E+10	-1.64E+11	-1.43E+22

Final Inverse (Multiply by 1/Determinant)

4.824E-11	-2E-17	-4.96E-17
4.583E-12	1.177E-06	5.874E-07
1.152E-11	-7.63E-07	-1.62E-06

Value of x1, x2, x3 after minus eror

x1	0.9518193
x2	0.4233887
x3	0.4204166

Figure 7. Calculation of coefficients using Newton-Raphson method

Equation to find value of x_4 and x_5

EFB $CH_{1.430}O_{0.615}$

Carbon balance:

$1 = x2 + x3 + x5$

Hydrogen balance:

$2w + a = 2x1 + 2x4 + 4x5$

Oxygen balance:

$w + b + 2m = x_2 + 2x_3 + x_4$

Variables	Number
x1	0.951819252
x2	0.423388705
x3	0.42041655
w	0.333333333

Calculation of x4 and x5

Variables	Number
x4	0.215723892
x5	0.156194744
m	0.050006533

Composition of Gas

$CH_{1.44}O_{0.66} + w\,H_2O + m O_2 + 3.76m\,N_2 = x1\,H_2 + x2CO + x3\,CO_2 + x4H_2O + x5\,CH_4 + 3.76m\,N_2$

Taking w= 0.2 and temperature of 800^{0}C

Assume 100 mol biomass inlet

Component	Outlet mol	Percentage of outlet(%)
H2	95.18192524	44.48078151
CO	42.33887054	19.78596299
CO2	42.04165505	19.64706711
CH4	15.61947442	7.299352551
N2	18.80245633	8.786835841
Total	213.9843816	100

Figure 8. Gas composition calculation (Step 3).

3.4. Model Validation (Step 4)

The synthesis gas compositions is compared with EFB gasification experimental data at temperature of 700°C where RMSE of 0.6173 is obtained. In order to further validate the developed thermodynamic equilibrium model, RMSE at different gasification temperature from 650 to 900°C are calculated where RMSEs lesser than 1 have been obtained at all investigated temperature as shown in figure 9. This indicates the thermodynamic equilibrium model is indeed reliable for representing gasification process.

Synthesis gas composition (%mol dry basis)	Raw EFB		
	Present model	Experimental data	RMSE
H_2	16.31	15.67	0.6173
CO	33.02	32.64	
CO_2	42.16	43.08	
CH_4	8.60	8.62	

Feedstocks	Gasification Temperature (°C)	RMSE
Raw EFB	650	0.5812
	700	0.6173
	750	0.7348
	800	0.8537
	850	0.8892
	900	0.8609

Figure 9. Model validation (Step 4).

3.5. Performance Evaluation (Step 5)

Lastly the gasification performance is evaluated based on synthesis gas compositions at different gasification temperature as shown in figure 10. Overall, a good agreement has been obtained between predicted values and the experimental data of synthesis gas for EFB indicating that the thermodynamic equilibrium model used in this work is able to predict the synthesis gas compositions accurately. The amount of hydrogen gas produced has increased from 14.65 mol% to 29.4 mol% when the gasification temperature is increased from 650°C to 900°C as shown in figure 10. Meanwhile the carbon monoxide composition has also increased from 30.56 mol% to 44.1 mol%. However, the amount of carbon dioxide and methane show an opposite trends as shown in figure 10. At gasification temperature of 650°C around 44.44 mol% of carbon dioxide composition have been produced and the amounts have decreased to 19.5 mol% when the gasification temperature is increased to 900°C. In the same condition the methane gas composition has initially produced approximately 9.72 mol% but has decreased to 5.8 mol%. The increment of carbon monoxide and hydrogen gas compositions can be explained through Boudouard reaction, water gas reaction and water gas-shift reaction as shown in Equations (3) – (5) respectively.

$$C + CO_2 = 2CO \quad (3)$$

$$C + H_2O = CO + H_2 \quad (4)$$

$$CO + H_2O = CO_2 + H_2 \quad (5)$$

As gasification temperature is increased, Boudouard and water gas reactions become more dominant and thus produce more carbon monoxide and hydrogen gas compositions. At low temperatures, carbon monoxide reacts with steam from moisture content of feedstock to produce both hydrogen and carbon dioxide gases. However, at higher temperatures, the water gas-shift reactions is shifted from right to left where carbon monoxide and steam are produced due to the consumption of hydrogen and carbon dioxide gases. Consequently, the amount of carbon dioxide and methane gases are decreased in order to produce carbon monoxide and hydrogen gases as the gasification temperature is increased.

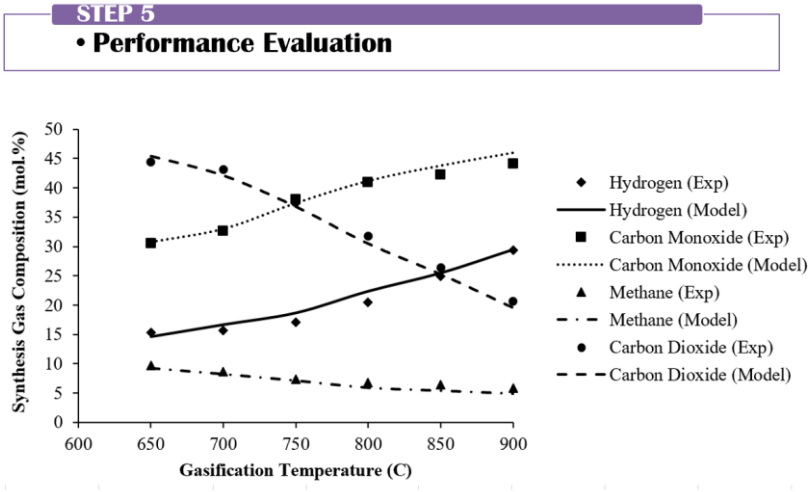


Figure 10. Performance Evaluation (Step 5).

4. Conclusions and Future Perspectives

The gasification model based on thermodynamic equilibrium approach has been integrated in Excel software for studying the gasification process. The database contain biomass properties has been integrated within the software for covering a wide range of biomass as feedstock for gasification process. The applicability of this software has been highlighted in gasification of EFB using air as gasifying agents. A good agreement has been obtained between predicted and experimental data where RMSEs lesser than 1 have been obtained at different gasification temperature. Based on the effects of gasification temperature, it was found that temperature of 900°C produces a highest hydrogen gas production at 29.4%. Although the software can be used to evaluate the effects of gasification temperature for a wide range of biomass but the gasifier's performance is not considered in this work. The performances of gasifier in terms of cold gas efficiency (CGE), lower heating value (LHV) and carbon conversion (CC) are essential in determining the suitability of the biomass as the feedstock for gasification process. In addition, the biomass database developed in this work consists only the raw biomass where some of the biomass have high moisture content and low carbon content. This ultimately reduces the production of synthesis gas. Due to the low carbon content and high moisture content, a further pre-treatment is recommended to improve the properties of biomass before it can be used for the gasification process. One of the pre-treatment methods that can be used is by using the torrefaction process where the moisture content will be significantly reduced and the carbon content as well as the calorific value will be increased [1, 15]. The addition of torrefied biomass in this developed software could provide a good alternative for biomass utilization as energy generation. This could represent the future direction of this work.

References

[1] Kuo P, Wu W and Chen W 2014 Gasification performances of raw and torrefied biomass in a downdraft fixed bed gasifier using thermodynamic analysis *Fuel* **117** 1231-1241

[2] Wahid F R A A, Muslim M B, Saleh S and Samad N A F A 2016 Integrated gasification and fuel cell framework: Biomass gasification case study *ARPN Journal of Engineering and Applied Sciences* **11(4)** 2673-2680

[3] Chen W H, Lin B J, Lee H M and Huang M H 2012 One step synthesis of dimethyl ether from the gas mixture containing CO2 with high space velocity *Appl Energ* **98** 92-101

[4] Ngamchompoo W and Triratanasirichai K 2017 Experimental investigation of high temperature air and steam biomass gasification in a fixed bed downdraft gasifier *Energ Source Part A* **39(8)** 733-740

[5] Madadian E, Orsat V and Lefsrud M 2017 Comparative study of temperature impact on air gasification of various types of biomass in a research scale downdraft reactor *Energ Fuel* **31**

4045-4053
[6] Moni M N Z and Sulaiman S A 2012 Downdraft gasification of oil palm frond: Effects of temperature and operation time *Journal of Applied Sciences* **12(24)** 2574-2579
[7] Patra T K and Sheth P N 2015 Biomass gasification models for downdraft gasifier: A state-of-the-art review *Renew Sust Energ Rev* **50** 583-593.
[8] Fortunato B, Brunetti G, Camporeale S M, Torresi M and Fornarelli F 2017 Thermodynamic model of a downdraft gasifier *Energy Convers. Manag.* **140** 281-294
[9] Muslim M B, Saleh S and Samad N A F A 2017 Torrefied biomass gasification: A simulation study by using empty fruit bunch *MATEC Web of Conferences* **131** 03008
[10] Muslim M B, Saleh S and Samad N A F A 2017 Effects of purification on the hydrogen production in biomass gasification process *Chemical Engineering Transactions* **56** 1495-1500
[11] Azzone E, Morini M and Pinelli M 2012 Development of an equilibrium model for the simulation of thermochemcal gasification and application to agricultural residues *Renew. Energy* **46** 248-254
[12] Karmakar M K and Datta A B 2011 Generation of hydrogen rich gas through fluidized bed gasification of biomass *Bioresour Technol* **102(2)** 1907-1913
[13] Hian G G, Saleh S and Samad N A F A 2016 A generic thermodynamic equilibrium model-based framework for biomass gasification processes *ARPN Journal of Engineering and Applied Sciences* **11(4)** 2222-2229
[14] Wahid F R A A, Harun N H H M, Rashid S R M, Samad N A F A and Saleh S 2017 Physicochemical property changes and volatile analysis for torrefaction of oil palm frond *Chemical Engineering Transactions* **56** 199-204
[15] Harun N H H M, Wahid F R A A, Saleh S and Samad N A F A 2017 Effect of torrefaction on palm oil waste chemical properties and kinetic parameter estimation *Chemical Engineering Transactions* **56** 1195-1200
[16] Robert H P and Don W G 1984 Perry's Chemical Engineers' Handbook 6th edition New York: McGraw Hill