Using a Simple Modeling and Simulation Scheme for Complicated Gasification System

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Abstract- Gasification processes are complicated with numerous parameters. It makes us difficult to understand the whole process nature. Therefore, a simplified approach based on modified stoichiometric equilibrium model for downdraft gasifier is designed in order to simulate the overall gasification process. The model uses the chemical reactions and species involved, while it starts by selecting all species containing C, H, O and N. Mass and energy balances of the gasifier -coupled with two equilibrium reactions are incorporated to create the model. This model can be solved with user friendly Micorsoft Excel and nonlinear Matlab solver. To validate the model, a close agreement is shown between numerical and experimental results within the same configuration. It can predict the composition of producer gases and heating values with acceptable accuracy. After validation, it is simulated to study the effects of temperature, moisture content of biomass and air-fuel ratio (related to equivalence ratio) in the downdraft gasifier. And then, experiments are conducted using optimized simulation data obtained from the model and it was found that the output producer gases were a close agreement with model results in producer gas composition and heating value.

Index Terms- Biomass, thermodynamic equilibrium model, downdraft gasifier, producer gas, parametric study

I. INTRODUCTION

Thermo chemical gasification is a process for converting solid fuels into gaseous form. The chemical energy of the solid fuel is converted into both the thermal and chemical energy of the gas. The chemical energy contained within the gases is a function of its chemical composition. Thus the composition of the product gas determines its quality as a fuel. High concentrations of combustible gases such as H_2 , CO and CH_4 increase the combustion energy of the product gas. During gasification, the organic material contained in the fuel is thermally released leading to the formation of porous char, which primarily consists of carbon and ash. The char particles undergo further reactions with several gases to yield the desired gaseous products. Thus thermo chemical characteristics of biomass play a major role in the selection of the gasification system design and performance.

Biomass gasification allows the conversion of different biomass feedstock to a more convenient gaseous fuel that can be used in conventional equipment (e.g., boilers, engines and turbines) or advance equipments (e.g., fuel cells) for the generation of heat and electricity. In addition to the production of heat and electricity, the product gas can be used to produce transport fuels such as synthetic diesel and hydrogen. Thermodynamic equilibrium calculations are suitable for studying the influence of fuel and process parameters to predict the potential synthesis gas yield and its composition without providing to the designer the appropriate gasifier dimensions. The gas composition is calculated assuming a fixed reactor temperature and that gasifier reactions are in equilibrium.

Biomass is one of the most promising renewable energy sources. It is in various forms and abundance in Myanmar. Biomass gasification is one of the effective technologies for its thermochemical conversion. The conversion is achieved by reaction between the feedstock and insufficient feed gas (air). The primary goal of biomass gasification is maximum energy conversion of the solid biomass into a combustible gaseous products known as producer gas. The quality of producer gas can vary as a function of gasifying agents (air, steam, oxygen) and the process operating parameters (gasification temperature, types of biomass).

Biomass gasifiers are complex equipments that require a lot of time to be mounted and to be put in operation; make it difficult to explore various working conditions. As a result, some mathematical models were made to predict the performance of the gasifiers. Thermodynamic equilibrium calculations are widely used in order to predict the thermodynamic limits of chemical reactions describing the gasification process. Since this approach is independent of the gasifier design, it is commonly used in studying the influence of important process parameters.

Zainal et al. (2001)[1]had studied an equilibrium model based on equilibrium constants to simulate the gasification process in a downdraft gasifier.

In the article by Barman et al.(2012)[2], the study used the applicable gasification reactions and also considered possible deviations from equilibrium to further upgrade the equilibrium model to validate a range of reported experimental results.

Mendiburu AZ, et al (2013)[3] used different equilibrium models for biomass gasification and validated one model by mean of universal RMSE(Root Mean Square Error) analysis method to be the more accurate and versatile among the four equilibrium models.

In order to predict the operation of a gasifier, the availability of a fairly simplified method to do it is important, and at the same time, it should be reliable and accurate. The chemical equilibrium model meets these prerogatives because it involves only thermodynamic parameters [4].

In this work, the existing equilibrium model of gasification process is modified by correlations and validated with existing published experimental results and models. After model validation, the model is used as a basis in order to predict the composition of the producer gas and its associated heating values by varying gasification temperature, moisture content of biomass and equivalence ratio.

II. EQUILIBRIUM MODELING

A zero dimensional model (time independent)(steady state) presented in this paper takes the advantage of thermo chemical equilibrium approach which is based on equilibrium constants.

A. Conforming a system of equation to model the downdraft gasification process

This model makes the following assumptions:

- 1. All reactions accounted are in thermodynamic equilibrium.
- 2. Species concentration and temperature are uniform throughout the chamber.
- 3. The gasifier chamber is perfectly insulated, with no heat transfer to the surroundings (Adiabatic).
- 4. Air entering the chamber is dry (relative humidity is zero), with 21% oxygen and 79% nitrogen by mass.
- 5. Steady state operation (time independent) is assumed.
- 6. The hard wood fuel may be represented by the chemical formula: $CH_{1.44}O_{0.66}[1,6]$
- 7. All the solid carbon is converted to syngas species and there is no solid carbon left after the gasification and the exit syngas is composed only of six gases in global model.
- 8. The gases estimated is free of any oxygen from the supplied air by partial oxidation and all oxygen is consumed during combustion reaction.

B. The global gasification reaction

All the equations that model the gasification process are developed on the basis of a proposed global gasification reaction. From the study of the gasification literatures and experimental works on downdraft gasifiers[1-9], the main species on the producer gas are carbon monoxide (CO),hydrogen (H₂), methane (CH₄), carbon dioxide(CO₂), water vapour(H₂O), nitrogen (N₂) and tars, while on the residues unconverted carbon (C) and ashes can be found.

On the side of the reactants, the feed biomass can be represented by a molecule comprising carbon (C), hydrogen (H), and oxygen (O) [1,6]. With the aforementioned consideration, the global gasification reaction considered in the present work is shown in Eq.(1)

$$CH_{1.44}O_{0.66} + wH_2O + m(O_2 + 3.76N_2) \rightarrow x_1H_2 + x_2CO + x_3CO_2 + x_4H_2O + x_5CH_4 + 3.76mN_2$$
(1)

Hard wood biomass (wet basis) represents $CH_{1.44}O_{0.66}+wH_2O$ and air is $O_2+3.76N_2$. x_1 to x_5 are the coefficients (mole/mole biomass) of respective permanence gases. In the global gasification, biomass is separated into $CH_{1.44}O_{0.66}$ formula and its moisture content fraction (w) in order to calculate effectively[1]. Because of the use of specified biomass formula, the model can be calculated on hard wood biomass only. The gasification agent can be air, oxygen and steam. In this system, air is primary interest.

C. Mass and energy balance

Atomic species balance is used to express the constraints of the system described as below:

C:
$$1 = x_2 + x_3 + x_5$$
 (2)

H:
$$2w+1.44=2x_1+2x_4+4x_5$$
 (3)

O:
$$w+0.66+2m=x_2+2x_3+x_4$$
 (4)

Energy balance is the importance boundary of this system and it is systematically reduced to:

$$\begin{array}{l} H^{\circ}{}_{f,biomass} + w(H^{\circ}{}_{f,H2O(l)} + H_{(vap))} = x_{2}H^{\circ}{}_{f,CO} \\ + x_{4}H^{\circ}{}_{f,H2O(vap)} + x_{5}H^{\circ}{}_{f,CH4} + \Delta T (x_{1}C_{pH2} + x_{2}C_{pCO} \\ + x_{3}C_{pCO2} + x_{4}C_{p H2O} + x_{5}C_{p CH4} + 3.76 .m .C_{pN2}) \end{array}$$
(5)

D. Modification of chemical equilibrium reactions

There are two methods in equilibrium modeling, stoichiometric and Gibb free energy minimization. In the present work, stoichiometric model is used and modified with experimental correlations to develop equilibrium model. The stoichiometric thermodynamic equilibrium modelling requires the use of equilibrium constants of each reaction considered in the model. An introduction to the thermodynamic equilibrium concepts can be found in [12].

In order to model the gasification process, the selected chemical reaction must be independent. The concept of independence of reactions states that if for many particular group of reactions one of them could be written as a combination of at least two of the others, then this group is not independent and the model may be computing recurrent information [10]. Using this concept, the two reactions: methane forming and water gas shift reactions were used to model the case without presence of unconverted carbon in the products.

Methane forming $C+H_2\leftrightarrow CH_4$ $K_1 = \frac{x_5}{x_1^2}$ (6) reaction(K₁₎ Water gas Shift $CO+H_2O$ $CO+H_2O$ CO_2+H_2 $K_2 = \frac{x_1x_3}{x_2x_4}$ (7) reaction(K₂)

The equilibrium constant (K) is a function of temperature only for each reaction considered and -RTlnK is equal to ΔG° where ΔG° is the standard Gibbs function of formation. From heat capacity, enthalpy and Gibbs free energy data from [11], equilibrium constants had calculated in the model. In pure equilibrium model, the equilibrium constants were far away from unity. Therefore responses were not suitable in practical case. So some experimental correlations were incorporated in this work.

The correlations -related to equilibrium condition used in the model are presented in equation (8) and (9) using from [1] and [2] respectively.

$$\ln K_{1} = \frac{7082.848}{T} - 6.567 \ln T + \frac{7.466 \times 10^{-3}}{2} T$$

$$-\frac{2.164 \times 10^{-6} T^{2}}{6} + \frac{0.701 \times 10^{5}}{2T^{2}} + 32.541$$
(8)

$$K_2 = \exp((4276/T) - 3.961)$$
 (9)

These two equilibrium correlations are the research works from the published papers.

III. MODEL IMPLEMENTATION

A. Model input

The inputs required for the model are as follows:

- 1. Fuel composition (using ultimate analysis and heating value of hard wood biomass [1])
- 2. Initial temperature of wood fuel and air (Ambient Temperature)
- 3. Equilibrium reaction temperature range (600-1000°C)
- 4. Equilibrium constants from the correlations[1-3] for the gasification reactions (Water gas shift reaction and Methane forming reaction)

Thermodynamic data for the chemical species involved - including enthalpy of formation (H^{o}_{f0}) , and coefficients for specific heat (C_{p}) [11].

B. Model output

The model outputs are producer gas compositions and heating values.Producer gas composition is the final gas composition that reflects thermodynamic equilibrium. Heating value can be calculated by using the combined heating values of carbon monoxide, hydrogen and methane composition.

C. Model implementation

The equations required for the numerical analysis are formulated using the C,H,O balance of the global equation followed by the rate constant equation for the two chemical reaction equations considered and finally carrying out the energy balance for the whole system.

The model is built within an Microsoft Excel work sheet. The MS Excel programming environment was chosen to make the model both user-friendly and portable. In the program, wood biomass is simplified to mole basis by using ultimate and proximate analysis of hard wood and heating values are calculated using correlations.

Using substitution and elimination, one linear and two nonlinear equations with three variables (x_1, x_2, x_3) are obtained and the set of equations is solved using nonlinear solver in Matlab. The system of one linear and two non-linear equations are solved by using fsolve (verifying with symbolic Matlab toolbox) in Matlab program to find the composition of hydrogen, carbon monoxide and carbon dioxide. The remaining variables are simultaneously calculated using the modified equilibrium constant correlations (6,7).Lower heating values are calculated using the heating value of carbon monoxide, hydrogen and methane on the dry basis.

D. Validation of the Model

The model was validated by the comparison with different experimental data in ref [4,5,7-9] and models developed in ref [3] using the universal testing method of root mean square error (RMSE) which was calculated as follow.

$$RMSE = \sqrt{\frac{\sum_{i=1}^{N} (experimental_i - Model_i)^2}{N}}$$
(10)

E. Comparison with experiment results

Comparative study was performed with the various experimental results obtained from the literature. The Table.1 below shows the comparison with experimental data from various references [4,7,8,9] and the current model. It could be observed that the model had some acceptable error (0.52 to 4.14) compared to experimental works. The comparison illustrated closeness between 5 proved the quantitative and qualitative validity of the present model for the parameters of interest.

	Exp[4]	Exp[7]	Exp[8]	Exp[9]	Model
H_2	14.00	19.38	17.50	15.23	13.19
CO	20.14	20.59	21.30	23.04	19.34
CO_2	12.06	11.67	13.30	16.42	15.46
CH_4	2.31	4.47	3.10	1.58	1.52
N_2	50.79	43.89	44.20	42.31	50.49
LHV	4.89	6.30	5.69	5.12	4.57
ER	0.30	0.27	0.30	0.30	0.30
RMSE	0.55	0.52	3.72	4.14	

TABLE I COMPARISON OF THE MODEL WITH EXPERIMENTS DATA FROM REF[4,7,8,9]

F. Comparison with models

TABLE II
COMPARISON OF THE MODEL WITH EXPERIMENT AND OTHER MODELS

	Exp[4]	M1	M2	M3	M4	Model
H_2	14.00	23.35	17.37	23.39	23.56	13.19
CO	20.14	25.24	22.86	19.47	25.47	19.34
CO_2	12.06	9.13	11.15	13.45	8.95	15.46
CH_4	2.31	0.72	3.81	1.15	0.58	1.52
N_2	50.79	41.56	44.80	41.53	41.45	50.49
LHV	4.89	5.97	6.13	5.76	5.97	4.57
ER	0.30	0.30	0.30	0.30	0.30	0.30
	RMSE	6.48	3.40	5.96	6.63	1.65

where

Exp[4]	=	Experimental results from ref.[4]
M1	=	Pure equilibrium model from ref.[3]
M2	=	Modification of equilibrium equations by
		multiplying with variables (α,β) from ref.[3]
M3	=	Modified by correlations from ref.[3]
M4	=	Modification of equilibrium equations from
		ref.[3]
Model	=	Current model

From the above comparison with different equilibrium models (Table-2), it was observed that the results predicted by the present model generally agreed with the reference models. It was shown that the model proposed had smaller variation of RMSE (1.65) compared to the previous equilibrium models (3.4~6.63). Considering that previous modelling efforts presented had been validated with RMSE value of at least 3.4 to 6.63, this model had only 1.65. This proves the worthiness of the present model.

IV. RESULTS AND DISCUSSION

A.Case study-1: Effect of gasification temperature on producer gas composition

After validating the model, it was used for the gasification of hard wood.

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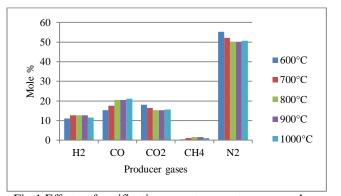


Fig.1.Effects of gasification zone temperature on producer gas concentration

The composition of producer gases from the model was calculated for a constant ER (0.3) and constant moisture content m (0.25) at $CH_{1.44}O_{0.66}$ within the different gasification zone temperature range 600-1000°C.

The results showed that hydrogen and methane compositions did not change sharply within the study range. But carbon monoxide and carbon dioxide percent changed significantly. By increasing the zone temperature, the carbon monoxide rose upward and carbon dioxide and nitrogen fell downward. Carbon dioxide and inert nitrogen are undesirable in the gasification system. So reducing these undesirables means achieving more percentage of combustible gases.

From the simulation results in Fig.2, gasification temperature range (800-900°C) gave the maximum heating value and it could be concluded that within the previous mentioned range(800-900), the maximum composition of combustible gases (H_2 , CO and CH₄) could be achieved from the gasifier.

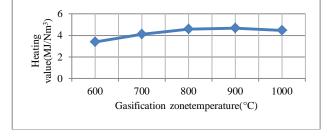


Fig.2. Effects of gasification zone temperature on heating value of producer gas at ER=0.3

Main targent of the optimization process is the maximization of the heating value of the producer gas. However it is essential to define the final use of the producer gas in order to further clear out and specify the goal of the process. For instance, if the producer gas will be used in an internal combustion engine, the heating value should be greater than 4.2 MJ/Nm³. The simulation result clearly showed that the reduction zone temperature should be greater than 700°C.

B.Case study-2: Effect of Moisture Content

The equilibrium model described above was used for the analysis on the gasification of hard wood.

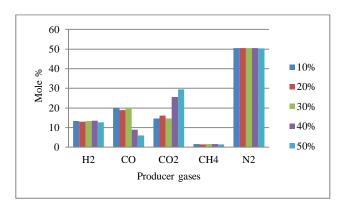


Fig.3. Effects of moisture content in wood on gas composition at $T=800^{\circ}$ C, ER=0.3

Fig.3 shows the effect of moisture content in wood on the composition of producer gas when the gasifier is working at 800°C and ER(0.3). It was observed that the composition of nitrogen and hydrogen was almost constant within the study range. Meanwhile, increasing moisture content of biomass, the content of carbon monoxide decreases sharply. CO content was very low at the range 40-50% moisture content. Inversely, the rise in carbon dioxide was found. And then, heating value of producer gas decreased rapidly, shown in Fig.4.Therefore, the effect of moisture content is very importent in gasification system to acquire sufficient heating value of producer gas.

In Fig.4, the heating values reduced significantly at moisture content >30%. So the simulation result also illustrates that maximum acceptable level of moisture content is 30% to be suitable in engine-generator set which has minimum limit of 4.2 MJ/Nm³.

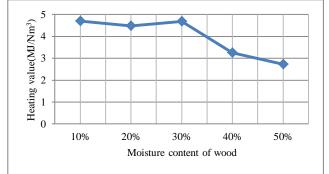


Fig.4. Effects of biomass moisture content on heating value of producer gas

C. Case study-3: Effect of Equivalence Ratio at $T=800^{\circ}C$ and w=0.25

Finally, effect of equivalence ratio on biomass gasification system had studied at T (800°C) and w (0.25) on hard wood biomass, shown in Fig-5and 6. By increasing ER, the important combustible gases decreased considerably and, on the contrary, nitrogen composition increased dramatically. Accordingly, heating value changed in a downward trend.

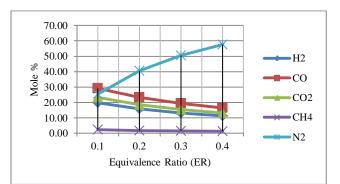


Fig.5. Effects of equivalence ratio in hard wood biomass on gas composition at T=800°C, w=0.25

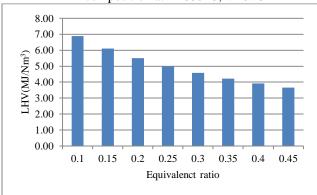


Fig.6. Effects of equivalence ratio in hard wood on gas composition at T=800°C, w=0.25

The results pointed out the theory of gasification. At combustion (oxidation) zone, the air is required to promote combustion of fuel. But, at gasification zone, the air is unfavourable for gasification (reduction) reactions.

V. COMPARISON WITH CURRENT EXPERIMENTAL GASIFIER

Experiments are carried out by construction of the pilot scale gasifier at Chemical Engineering Department, Yangon Technological University (Fig.7). The objective of gasifier experiment is to achieve sufficient heating value producer gases by using briquette rice husks. It consists of reactor insulated with fire clay, cyclone, water scrubber, foam filter, dolomite filter and gas holder. Blower is to monitor air flow rate into the system. Water pump is to scrub the producer gas for tar and particulate removal and cool the output gas. Recycle system of water was conducted and briquette rice husks were used in all experiments. Measuring devices used are k type thermocouples for temperature, anemometer for gas flow, water flow meter and GC–TCD for gas compositions and heating value measurement.

In experiments, there are various parameters to be optimized for sufficient heating value producer gas. Some observations beyond the scope of modeling work were described as follows:

- 1. Reactor had a problem in ash removal (causing bridging, combustion zone shift). That is because of manual grade handled from the top of the reactor.
- 2. Water Scrubber was important to eliminate tar from the producer gas and to cool gases. Without using it, the outlet producer gases were hot and considerable amount of tar and moisture are included in the product gas. This caused the product gas incombustible.

- 3. Dolamite ring and foams used in the two filters could effectively absorb moisture and tar from the producer gases.
- 4. Combustible gases with sufficient heating value for engine quality had found. Sometime, the combustible gases were unstable.



Fig.7. Experimental Gasifier System

In comparison with model parameters, because of instability nature of operation conditions mentioned above, the results are described as follows:

Temperature: :Although temperature is fixed in model, the real temperature distribution at pilot gasifier is changing time by time in the gasification zone within the range 700~1000°C. This is due to the unstable nature of gasification zone. This problem can be minimized by the continuous ash removal system. At present, manual grate is used in all experiments. In addition, temperature distribution is directly proportional to the air flow rate. As excess air favors complete combustion instead of gasification, careful adjustment of air flow is required for producer gas.

Moisture content: : In practical work, we used rice husk briquette which had moisture content <16%, so any problem related with it was not found. It is recommended that in rainy season proper drying of raw materials is required in sunlight for about one day before using in the gasifier.

Air-fuel ratio (ER): : It was controlled by the valves (before blower) in experiments, for ER calculation, it is still needed to install the flow measuring devices in 4 air nozzles.

So the current experimental works find difficulty to compare with the modeling scheme. But the modeling work shows that the objective of experimental work is combustible producer gas that is the driver of engine. The output producer gas components and their compositions in experiments are closely matched with the model outputs. Although the model cannot effectively compare the current experiments in the parameters, the objection function, producer gas quality and quantity, is comparable with the experiment work.

VI. CONCLUSION

An equilibrium model was developed and tested to study the influence of the three gasification process parameters, namely moisture content, equilibrium temperature and air fuel ratio. This model can be used in the downdraft gasification system with acceptable accuracy in producer gas composition and heating value. So the designer of the gasifier can use this simulation data in the optimization of moisture content of biomass, equilibrium gasification zone temperature and air-fuel ratio to control producer gas composition and heating values in order to fulfil the specific requirement (e.g. boilers, engine-generator set, further synthesis of chemicals, fuel cells, etc). The model is very simple and clearly provides the operating range of equivalence ratio, moisture content for the woody biomass and optimum gasification zone temperature. Furthermore, this model facilitates the prediction of maximum temperature in the gasification zone which provides useful information for the designing of the gasifier and the selection of material for the construction.

The merits of the model lies in the fact that it is capable of handling predictions for all category of biomass materials with wide operating range of equivalence ratio and moisture content in the gasifier.

In the experimental work, all sample gases contain hydrogen, carbon monoxide, carbon dioxide, methane and nitrogen. It was not found significant composition of other impurities such as tars. The lower heating values of producer gas were in the range 4.5 to 7 MJ/Nm³. So the experiment results show a close agreement with model output.

The model cannot be regarded at the actual gasification system but it gives useful information for designing the system such as choice of materials and clay for insulation, design of throat for gasification zone, air inlet control. Therefore more research work is required to assess the effects of operation conditions and feed stock properties (type, morphology, size distribution, density) on these factors.

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