

Thermodynamic Model for Updraft

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Research Article

Thermodynamic Model for Updraft Gasifier with External Recirculation of Pyrolysis Gas

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Most of the thermodynamic modeling of gasification for updraft gasifier uses one process of decomposition (decomposition of fuel). In the present study, a thermodynamic model which uses two processes of decomposition (decomposition of fuel and char) is used. The model is implemented in modification of updraft gasifier with external recirculation of pyrolysis gas to the combustion zone and the gas flowing out from the side stream (reduction zone) in the updraft gasifier. The goal of the model obtains the influences of amount of recirculation pyrolysis gas fraction to combustion zone on combustible gas and tar. The significant results of modification updraft are that the increases amount of recirculation of pyrolysis gas will increase the composition of H_2 and reduce the composition of tar; then the composition of CO and CH_4 is dependent on equivalence ratio. The results of the model for combustible gas composition are compared with previous study.

1. Introduction

The types commonly used in gasification are the fixed bed (updraft and downdraft) and fluidized bed. The updraft gasifier has many advantages but, on the other hand, produced high level of tar [1]. Several modifications to gasifier with recirculation of pyrolysis gas have been conducted to reduce the tar [2–4]. In previous study, we have modified type of updraft gasifier with pyrolysis gas recirculated externally to the combustion zone. Furthermore, the produced gas exits at the reduction zone (side stream) to reduce the tar [4].

Modeling is needed in the gasification process as a tool to predict the results that will be obtained from an experiment. Some thermodynamic modeling using Aspen Plus has been done before on updraft gasifier. Chen et al. conducted a model using one process of decomposition of MSW as fuel to see the effect of flue gases of combustion on the LHV; the results showed the flue gas will increase the LHV [5]. He et al. applied a model on Lurgi gasification process using one process of decomposition of coal as fuel to see the effect of oxygen/coal ratio on exergetic efficiency of the process;

the results of modeling showed oxygen/coal ratio affecting exergetic efficiency of the process [6]. Modeling generally only uses one process of decomposition using ultimate analysis of fuel. In this study, we use a model using two processes of decomposition (decomposition of fuel and char) using the ultimate analysis of fuel and char. The model is implemented on updraft gasifier with external recirculation of pyrolysis gas [4].

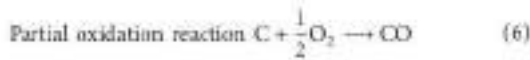
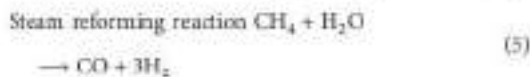
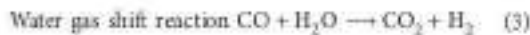
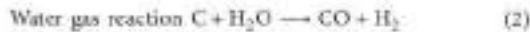
Modeling aims to get the effect of the amount of external recirculations of pyrolysis gas flow to the combustion zone on the composition of the combustible gas (CO, H_2 , and CH_4) and tar composition (C_7H_8O , $C_{10}H_8$).

2. Methodology

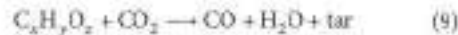
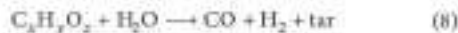
The process that occurs during the gasification includes drying, pyrolysis, reduction, and combustion; meanwhile each stage of the process results in a product for the next stage or directly results in a gasification process product. The processes of drying and pyrolysis are the processes that are not in an equilibrium state and may take place

instantaneously [7]. The composition of the product in its process is calculated using the mass and energy balance principles. The process of gasification and combustion is a process that can take place in an thermodynamic equilibrium state [8]. The composition of the product in thermodynamic equilibrium conditions can be calculated using Gibbs free energy minimization [9].

The reactions of combustion and gasification taking place at equilibrium conditions are as follows:



In this simulation process, tar is modeled as cresol and naphthalene. Cresol is to represent nearly approaching heavy tar and naphthalene to represent light tar [10]. Tar will experience reforming when entering the combustion and gasification zones to form H_2 and CO through the reaction of steam reforming and dry reforming [11]:



In equilibrium, the total Gibbs free energy (G_{total}) of the system is in a minimum state. The concentration of each compound (n_i) is obtained by minimizing the objective function G_{total} :

$$G_{\text{total}} = \sum_{i=1}^N n_i \Delta G_{f,i}^{\circ} + \sum_{i=1}^N n_i RT \ln \left(\frac{n_i}{\sum n_i} \right) \quad (10)$$

Limits for completion of the object function are expressed in the mass balance of elements:

$$\sum_{i=1}^N a_{ij} n_i = A_j, \quad j = 1, 2, 3, \dots, k \quad (11)$$

G_{total} is total Gibbs free energy, G_f° is standard Gibbs free energy, R is universal gas constant, T is temperature, N is number of compounds, a_{ij} is number of atoms in element number j in mole of compound number i , and A_j is number of atoms in element number j in mixture of reaction.

The Gibbs minimization equation can be solved using Lagrange multiplier:

$$L = G_{\text{total}} - \sum_{j=1}^k \lambda_j \left[\sum_{i=1}^N a_{ij} n_i - A_j \right] \quad (12)$$

where λ is Lagrange multiplier.

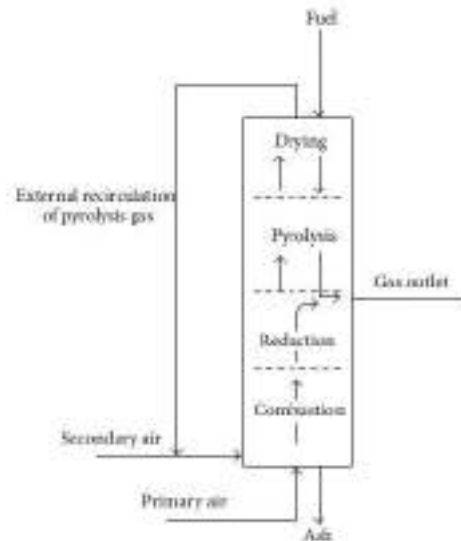


FIGURE 1. Updraft gasifier with external recirculation of pyrolysis gas [4].

Equilibrium conditions will be obtained if the partial derivative of the Lagrange function is zero:

$$\left[\frac{\partial L}{\partial n_i} \right] = \frac{\Delta G_{f,i}^{\circ}}{RT} + \sum_{i=1}^N \ln \left(\frac{n_i}{\sum n_i} \right) + \frac{1}{RT} \sum_{j=1}^k \lambda_j \left(\sum_{i=1}^N a_{ij} n_i \right) = 0 \quad (13)$$

Calorific value of gas resulting from the gasification process is calculated based on

$$\text{LHV (kJ/Nm}^3\text{)} = y_{\text{CO}} \cdot 12621 + y_{\text{H}_2} \cdot 10779 + y_{\text{CH}_4} \cdot 35874 \quad (14)$$

Modeling starts with the approach to the process of experiments that have been carried out by Surjosatyo et al. [4] as shown in Figure 1. Furthermore, the approaches are used to facilitate the simulation process. The approach is taken to the gas flows out from the gasifier at the end of the pyrolysis process, so that, in modeling, the fraction of the pyrolysis gas uncirculated does not enter the equilibrium zone and directly goes out of the reactor (Figure 2). Primary air and secondary air in the experiment are the total quantity of air for the combustion process, so that, in modeling, the total quantity of air only is used to enter the equilibrium zone.

Modeling is developed by applying the mass and energy balance as well as the Gibbs free energy minimization in the configuration of the updraft gasifier reactor with an external recirculation of pyrolysis gas as described in Figure 1. The mass and energy balance are used in the stages of drying, pyrolysis, reduction, and combustion processes. Gibbs free energy minimization is used during the combustion and

TABLE 1: Proximate and ultimate analysis of fuel.

	Unit	Value	Normalization
Proximate analysis			
Moisture	Mass fraction (%)	10.24	
Ash	Mass fraction (%)	2.71	
Volatile	Mass fraction (%)	71.80	
Fixed carbon	Mass fraction (%)	15.25	
Ultimate analysis (dry basis)			
Carbon	Mass fraction (%)	43.33	48.27
Hydrogen	Mass fraction (%)	5.11	5.69
Oxygen	Mass fraction (%)	38.61	43.01

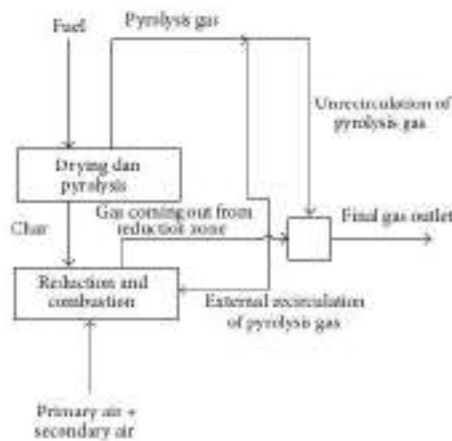


FIGURE 2: Configuration model updraft gasifier with external recirculation of pyrolysis gas.

reduction (gasification) processes to obtain the product composition.

Modeling of the pyrolysis zone is a process of decomposition of nonconventional fuel elements into the conventional compound [12]. The conversion process is facilitated by using proximate and ultimate analysis data available in Table 1 which is further decomposed into its conventional compounds as presented in Table 2. The conventional data could be compared to the data of literature obtained by Wang et al. [13] and Milh e et al. [14] as presented in Table 3. It shows tendency of the same distribution of the composition.

Modeling in the reduction and combustion zones is performed using proximate and ultimate analysis data of char. The proximate and ultimate analysis data of char is decomposed into its conventional compound. The product of decomposition is mixed with the pyrolysis products and combustion air. The mixture then enters the thermodynamic equilibrium reactions in the process of gasification and combustion.

The ratio of the amount of gas resulting from the process of pyrolysis recirculated to enter the combustion chamber to the total amount of gas resulting from the pyrolysis process

TABLE 2: Pyrolysis product (fuel decomposition).

Compound	Mass (kg)	Mass fraction
CO	0.49	0.10
CH ₄	0.09	0.02
H ₂ O	1.79	0.36
CO ₂	0.51	0.10
C ₇ H ₈ O (tar)	0.76	0.15
C ₁₀ H ₈ (tar)	0.36	0.07
Char	0.88	0.18
Ash	0.12	0.02

TABLE 3: Pyrolysis product of wood [13, 14].

Species	Mass fraction (%) [13]	Mass fraction (%) [14]
Gas	64.8	51
Pyrolysis water		26
Tar (organic compound)	20.0	15
Char	15.2	21

is called the fraction of the pyrolysis gas recirculating. The fraction of pyrolysis gas recirculation is a variable that is used to see the effect of pyrolysis gas recirculation on composition of combustible gas (CO, H₂, and CH₄) and tar (C₇H₈O and C₁₀H₈). Modeling carried out under operating parameters is presented in Table 4.

Modeling is performed using Aspen Plus Simulator. The process that occurs in the drying and the pyrolysis zone simulated using RYield reactor block [7, 15] and the processes in the zone of combustion and gasification are modeled using RGibbs [8, 16]. Thermodynamic properties are calculated using the state equation of Peng-Robinson. The enthalpy and density of nonconventional component are calculated using the models of HCOALGEN and DCOALIGT.

3. Results and Discussions

3.1. The Effect of the Fraction of Pyrolysis Gas Recirculation. Figure 3 presents the results for simulating the effect of the fraction of pyrolysis gas recirculation to the combustion zone

TABLE 4: Simulation parameters.

Number	Parameter	Value
1	Stoichiometric combustion air (kg/h)	25.6
2	Fuel flow rate (kg/h)	5
3	Equivalence ratio (ER)	0.2–0.4
4	Pyrolysis gas recirculation fraction	0–1

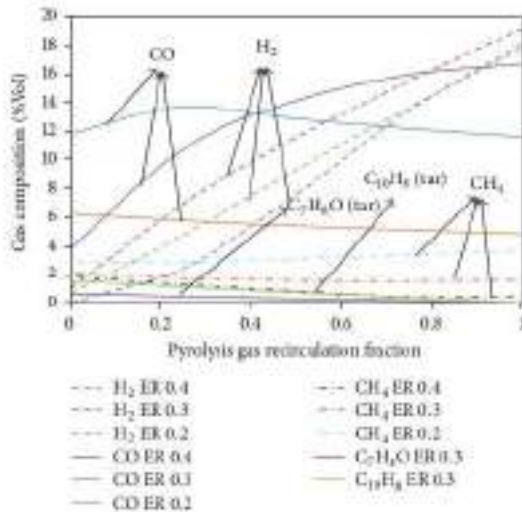


FIGURE 3: Gasification product according to pyrolysis gas recirculation fraction and equivalence ratio.

on the combustible gas (CO, H₂, and CH₄) and tar (C₇H₈O, C₁₀H₈).

H₂ concentration increases by the addition of pyrolysis gas recirculation flow fraction for each equivalence ratio due to the greater amount of water vapor and tar carried away by the flow of pyrolysis gas. The reactions contributing to increasing H₂ are the water gas reaction, water gas shift reaction, and steam reforming tar reaction. The modeling results show the same trend as the experimental results [3, 4, 17, 18]. The increase in equivalence ratio from 0.2 to 0.3 tends to increase the concentration of H₂ but in the equivalence ratio above 0.3 will reduce the composition of H₂. This is because of a shift in reaction to the Boudouard reaction and reverse water gas shift due to the increase in heat of combustion. The maximum concentration of H₂ is obtained on the condition that the amount of pyrolysis gas recirculation flow is maximum (pyrolysis gas recirculation flow fraction of 1).

CO concentration tends to decrease by the increase in the fraction of pyrolysis gas recirculation flow until the equivalence ratio reaches 0.3 and then will increase. The modeling results show the same tendency as the experimental results [3, 4, 17, 18]. This is due to increasing Boudouard reaction which is influenced by the increase in the heat released by the combustion process and CO₂ carried by the pyrolysis gas.

CH₄ concentration tends to increase by the increase in the fraction of pyrolysis gas recirculation flow until the equivalence ratio reaches 0.2 and then will decrease. This is because, in the equivalence ratio below 0.2, the methanation reaction takes place better as it is an exothermic reaction. The addition of pyrolysis gas will increase the amount of H₂ for the methanation reaction. CH₄ carried by the fraction of pyrolysis gas recirculation flow also contributes to the increase of CH₄. In the equivalence ratio above 0.2, the methanation reaction will decrease by the increase of heat released on combustion reaction. CH₄ in the pyrolysis gas will react with H₂O to produce H₂ through steam reforming reaction.

The tar content in the producer gas decrease by the increase in fractions of pyrolysis gas recirculation flow to the combustion zone as presented in Figure 3. This is because the tar experiences decomposition through the reforming process into H₂ and CO as it receives heat resulting from combustion process.

The pyrolysis gas recirculation flow fractions of zero (0) and one (1) represent each of the updraft and downdraft operations. The difference in the operating condition leads to significant difference in composition of combustible gas and tar, especially the concentration of H₂. It shows the significance of the effect of H₂O (water vapor) and tar contents in the pyrolysis gas on H₂ concentration. Research by Ueki et al. [19] and Saravanakumar et al. [20] presents a direct comparison between the operation of the updraft and downdraft gasifier or crossdraft gasifier. The results show there is a large difference in concentration between H₂ and tar.

The simulation results show that the variation of pyrolysis gas recirculation fraction gives an influence on the composition of the combustible gas and tar. Therefore, its variables are very important to do the experiment until the fraction of the pyrolysis gas recirculation flow reaches maximum.

3.2. The Effect of Equivalence Ratio. In the condition where the recirculation flow fraction is maximum (pyrolysis gas recirculation fraction of 1) as shown in Figure 4, an increase in the equivalence ratio will increase the concentration of H₂ until equivalence ratio of 0.3 and CO until equivalence ratio of 0.4 and then it will decrease. This is because the process will move towards the stoichiometric combustion where more heat is released. The increase in heat causes the Boudouard and the water gas reactions to be better. However, under a certain condition, its reaction will decrease because of the decrease of char quantity to produce heat when it burns a lot by the addition of the air supply (an increase of equivalence ratio) [21]. An increase in the equivalence ratio reduces the concentration of CH₄. It is caused by a decrease in methanation reaction. Methanation reaction is a reaction that releases heat; therefore it will be dominantly in the lower equivalence ratio. The results of model have a similar tendency with model results reported by Doherty et al. [7], Paig-Arnavat et al. [21], and Reed and Das [22], especially for Reed and Das model in which H₂ seems to continuously decrease. This is because in this modeling there is a heat loss.

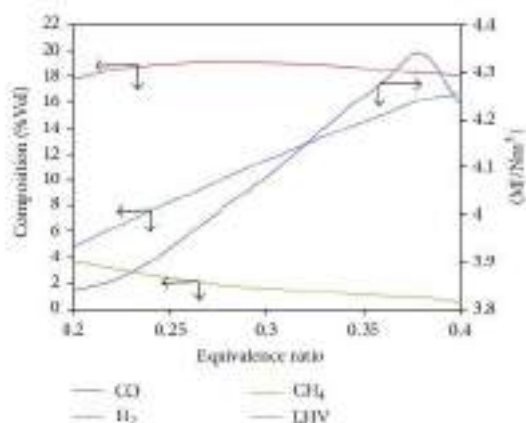


FIGURE 4: Combustible gas and LHV according to equivalence ratio at the maximum pyrolysis gas recirculation fraction.

TABLE 5: Comparison between models and experiments for gas composition in ER 0.3 and fraction of pyrolysis gas recirculation of 0.5.

Combustible gas	Model (% mol)	Experiment (% mol)	Error (%)
CO	12.8	14.4	11.1
H ₂	11.5	14.93	22.9
CH ₄	1.6	3.49	54.1

The simulation results in equivalence ratio of 0.2 to 0.4 at the maximum pyrolysis gas recirculation flow which results in a high LHV. In the experiment, it is necessary to select a mechanism that can discharge the pyrolysis gas recirculation flow maximum with total combustion air between 0.2 and 0.4 of stoichiometric air.

The LHV maximum of 4.34 MJ/Nm³ is in the equivalence ratio of 0.38. The simulation shows the best operating condition which occurs in the equivalence ratio of 0.38 with a fraction of the maximum pyrolysis gas flow. This condition would provide the highest value of LHV and the lowest of tar.

3.3. Comparison between Simulation and Experiment. Comparison of the results of simulations and experiments which have been conducted by Surjosatyo et al. [4] is presented in Table 5. The results of the comparison show a trend of values which are almost equal to the concentration of CO and H₂. The CH₄ composition shows a bit far different value. The difference in the CH₄ value is almost equal to that obtained from thermodynamic modeling carried out by Kuo et al. [8], Jarunghammachote and Dutta [23], and Barratieri et al. [24]. This is because the CH₄ final product is affected by factors beyond the equilibrium (nonequilibrium). Thus, it cannot be predicted purely thermodynamically [24].

In general, the results of the simulation show lower values, because the parameters in the simulation are still different to the experimental condition.

4. Conclusions

The simulation results show that an increase in the fraction of the pyrolysis gas recirculation flow will affect the composition of the combustible gas and tar.

The concentration of H₂ increases in each equivalence ratio constant. The concentration of CO decreases until the equivalence ratio reaches 0.3 and increases above that. The concentration of CH₄ increases until the equivalence ratio reaches 0.2 and decreases above that.

The composition of C₇H₈O (tar) and C₁₀H₈ (tar) decreases by the increase in the fraction of pyrolysis gas recirculation flow into the combustion zone.

The best operating condition exists when the amount of recirculated flow is maximum (pyrolysis gas recirculation flow fraction of 1) and the equivalence ratio is 0.38.

Modeling and experimental results show a tendency to approach the same value, especially composition of CO and H₂.

Conflict of Interests

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

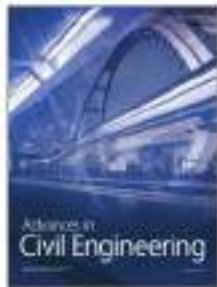
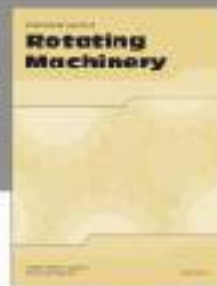
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