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Performance modelling and validation on co-gasification of coal and sawdust pellet in research-scale downdraft reactor

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Abstract. Co-gasification of the fossil fuel with the biomass is considered a very promising clean energy opt-in reduce the greenhouse gas emission. The main objective of this research is to develop a simple and reliable model provided as a preliminary tool to evaluate the performance of the co-gasification of sub-bituminous coal with densified biomass (sawdust pellet, SP). The simulation model using Aspen Plus was validated with the experimental data for minimization of the Gibbs free energy model. Three performance parameter; the calorific value of the syngas (CV_{syngas}) , syngas yield (Y_{syngas}) and gasification efficiency (ηGE) were studied along with three different control parameter. The increase of the sawdust pellet blending ratio denoted in a decrease of the CV $_{syngas},$ Y $_{syngas}$ and ηGE ranged from 3.00-6.00 MJ/Nm³, 1.20-2.20 Nm³/kg and 25%-37%, respectively. On the contrary, effect of the gasification temperature at the various blending ratio exhibits an increase for all the performance parameters. In addition, ERair resulted in the decline of the CV_{syngas} from 8.50 to 1.58 MJ/Nm³ and ηGE from 52 to 15% while vice versa for Y_{syngas}. Furthermore, it is found that the result obtained from the developed model agrees well with the experimental data that have been conducted in replicate.

1. Introduction

Rapidly rising on the issue of depletion of fossil fuels together with the production of greenhouse emissions during the energy production, eventually causing global warming and acid rain [1]. Thus, it has heightened the need to search for promising solution that is renewable, environmentally friendly, sustainable, economically, and lessen the current environmental issues. Recent research has proven that co-utilization of coal and biomass has been a development of sustainable bioenergy network between a renewable and non-renewable resource, especially in the co-gasification to produce syngas and electricity in a sustainable manner [2]. Co-gasification technology aids in reduces potentially the exploitation of a significant amount of conventional coal resources, assists in lower the greenhouse gases (GHG) emissions, but also boost the overall gasification process efficiency [3]. It has been discovered that the co-gasification of these two fuels exhibits synergism reaction that reduces the GHG emission without deprived the energy content of the product gas [4]. Furthermore, biomass characterization and the percentage mixture of the biomass with coal play an essential role as it is directly associated with

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the fuel gas composition. The co-gasification process between biomass and fossil fuels significantly produce low carbon footprint on the environment and enhance the H_2/CO ratio in the produced syngas, which is essential in liquid fuel synthesis. Another crucial point, it has been discovered that the inorganic matter present in biomass functioning as a catalyst for the coal gasification [5]. Thus, production of the superior gas quality by using coal-biomass blends at different operating condition of temperatures and equivalence ratio of air have gained interest among the researchers [6]. Several numbers of research on co-gasification of the various blending ratio of biomass with the coal have been conducted by with the result indicates that blending coal with biomass eventually enhances the gasification with beyond levels that impossible to be achieved by gasifying these feedstocks alone [7]. Most of the studies were focused on the raw biomass co-gasified with coal; however, the co-gasification on the pre-treated biomass, especially, palletization still lacks. Dafnomilis et al. [8] expressed the opinion that the pre-treated of the biomass in the form of pelletized or otherwise densified resulted in better fuel operability in term of handling, transportation, storage, and feeding compared than raw biomass. Gasification of pellet fuel has widely been applied in the commercial gasification resulted that the syngas composition is much more stable by maintaining the gasification more steady and efficient; the uniform shape and density of the pellet fuels aid in smooth feeding by making less of a biomass bridge and gasification reactions [9]. It has been discovered a number of researches have been found on the co-gasification of biomass pellets/coal conducted with the results promised an efficient production of syngas. Although, the pelletized biomass has been utilized as a co-feed in gasification or combustion system; however, the reason for the improvement in the efficiency of the pelletized case gasification is not apparent [10]. The development of fuel-flexible gasification in the pellet form co-gasified with coal remains a challenge, and the field requires further attention. Hence, this study attempt to simulate co-gasification model of the downdraft fixed bed gasifier with the application of the Aspen Plus® software environment.

Numerous researches have been conducted the modelling of the downdraft gasification on various feedstock either using the agriculture residue or forestry residue. This is due to the application of the software that serves as a suitable alternative to minimize the experimental cost and time [11]. Simulate the gasifier by breaking gasification into the drying zone, the pyrolysis zone, the oxidation zone and the reduction zone as well as considered the heat and mass transfer in the model; this tool is capable of predicting gasification performance effectively. Subsequently, the performance of a gasifier system at the different operating and design parameters which can be validated from the optimal model allows designers to speculate the effects of parameters even without any further experimental data [12]. Keche et al. [13] built the developed model with the different biomass fuels in an atmospheric fixed bed reactor to investigate the syngas composition. A model develops by Gao et al. [14] investigated the production of hydrogen gas from the co-gasification of coal and biomass in the presence of calcium oxide as a sorbent. Co-gasification of the charcoal with empty fruit bunch also being developed by Monir et al. [11] which found out that the highest mole fraction of H_2 and CO occur at 975 °C and 35 bar. Ali et al. [3] develop a simulation model of the rice-husk and coal that indicated the model capable of serving as a reliable benchmark for revamping an existing Egyptian natural gas-based power plant. Kuo and Wu [15] design the co-gasification of the coal with the pre-treated biomass, which is the torrefied woody biomass as the substitutions to the raw woody biomass. The simulation denoted that the utilization of the torrefied woody biomass significantly improves syngas yield. Meanwhile, according to the power generation's view, the co-gasification of coal and torrefied biomass resulted in an optimal input condition in terms of power generation and system efficiency. As far as the authors are aware, there are still limited works on modelling of coal co-gasification with pre-treated biomass, especially densified biomass using ASPEN Plus software.

Therefore, the objective of this study was to investigate the co-gasification of sub-bituminous coal (CL) with sawdust pellet (SP) by modelling and simulate a kinetic free equilibrium model of fixed-bed downdraft gasifier in Aspen Plus. The sawdust pellet (SP) blending ratio, gasification temperature and air equivalence ratio were varied to predict the calorific value of the syngas (CV_{syngas}), syngas yield (Y_{syngas}) and gasification efficiency (η GE). Furthermore, the results obtained from the experimental measurement was used to verify the simulation results. The results acquired through this study is served for preliminary investigating on gasification performance of the pre-treated biomass co-gasified with coal.

2. Methodology

2.1. ASPEN Plus simulation model

In modelling the co-gasification process, a kinetic free equilibrium model was developed using ASPEN Plus software (ver. 8.6) by including the major chemical reactions occurring in the gasifier. The co-gasification process was divided into three sub-systems to form a downdraft gasifier system. The drying sub-system is to minimize the moisture content of the feed before being fed into the next reactor. The second sub-system aids in decomposed the feed into volatile components and char. Moreover, a FORTRAN statement was included to specify the yield distribution for each conventional component. Next, the RGibbs sub-system simulated the partial oxidation and gasification process by minimizing Gibbs free energy. In carrying out the modelling, some assumptions were made. The assumptions applied in the model were:

- The process occurs in a steady state with kinetic free and the residence time is not considered.
- Atmospheric pressure was assumed in all sub-system.
- Air was introduced in the RGibbs to enhance the co-gasification process at ambient temperature and pressure.
- The gasification agent mixed homogenous and reacted with feed instantly in the reactor.
- All sulfur produced in the H₂S form; meanwhile no oxide of nitrogen was formed as only NH₃ produced.
- Tars are assumed to be negligible in the syngas.

The gases involved are in compliance with the Peng-Robinson equation of state with Boston-Mathias alpha function (PR-BM) to estimate all physical properties of the conventional and non-conventional components at the multiple phase in the gasification process [16].

2.2. Model development

The simulation model flowsheet used in the developed model is shown in Error! Reference source not found. Firstly, the stream of feed consists the mixture of sawdust pellet and coal, with their blends of a ratio of 0, 25, 50, 75, 100% w/w, respectively were fed into the system. Sawdust pellet blending ratio was defined as the mass ratio of sawdust pellet to the total of biomass and coal, therefore, 0, 100% of sawdust pellet blending ratio refers to the pure coal and pure sawdust pellet, respectively. The feed stream was passed through all block with different reaction temperature. The feedstock was specified as a non-conventional component in Aspen Plus was defined by their ultimate and proximate analysis present in Table 1. In additional, Table 2 provides the operation model that was used in this study. Drying process that removes the residual moisture in the feed was simulated in the 'RStoic' block by including the FORTRAN statement in the calculator block to control the drying operation. After drying, the feed was then decomposed into its components constituent (C, H, O, S and N) by specifying yield distribution in the block 'RYield'. In the 'RYield' block, the yield distribution of the feed was specified by FORTRAN statement in a calculator block into its components. The total yield of volatiles was assumed to be equal to the volatile content of the parent fuel by taken into account the proximate analysis of the fuel. The co-gasification process was simulated in 'RGibbs' block by minimizing the Gibbs free energy assumed the complete chemical equilibrium calculations. The gasifying agent, which is air, was introduced into the block where partial oxidation and gasification reactions take placed. Furthermore, the 'RGibbs' block also capabled of calculating the syngas composition as it can generate light gases such as CO, CO₂, H₂, H₂O, N₂, CH₄, and H₂S. The outlet stream of the 'RGibbs' was passed through the 'Sep' block to separate gases from ash according to the specified splits fractions as desired.



Figure 1. ASPEN Plus simulation model of co-gasification on coal and SP.

Components	Coal (CL)	Sawdust Pellet (SP)	
Proximate analysis (wt %)			
Moisture content	8.18	9.19	
Volatile matter	39.79	79.00	
Fixed carbon	33.81	10.16	
Ash content	18.22	1.65	
Ultimate analysis (wt %)			
Carbon (C)	52.58	44.28	
Hydrogen (H)	5.90	6.09	
Nitrogen (N)	1.49	1.05	
Sulphur (S)	1.14	0.28	
Oxygen (O)	38.90	48.62	
Calorific value (MJ/kg)	20.19 ± 0.082	17.46 ± 0.085	

Table 1. Proximate, ultimate and calorific value of the coal and SP.

 Table 2. List of ASPEN Plus unit operation model.

Aspen Plus Model	Operation	Description	Function	
RStoic	Drying	Conversion reactor with known stoichiometry	Reduce the moisture content of the wet feed	
RYield	Decomposed	Yield reactor with known products yield	Decomposed non- conventional feed into its element constituents applying FORTRAN statement	
RGibbs	Gasifier	Multiphase chemical equilibrium reactor (non- stoichiometry)	Models gas-phase chemical equilibrium and aids in calculating the syngas	

Aspen Plus Model	Operation	Description	Function
			composition by minimizing Gibbs free energy
Sep	Separator	Split a stream into two stream or more by specifying split fractions	Separates gas from ash

2.3. Model verification

In order to demonstrate the validity of the proposed model, the experimental measurement of cogasification of coal with SP displayed in Figure 2 was carried out in a lab-scale electrical downdraft gasifier, as shown in Figure 3.



Figure 2. Image of coal (a) and SP (b) that have been used in this study.

The system was custom-fabricated and located in the Biomass laboratory under the Department of Mechanical Engineering of Universiti Teknologi Petronas, Malaysia. The reactor is a cylindrical tube made up of stainless steel class SS316 consist of an internal diameter of 80 mm and 500 mm long. The gasifier was positioned vertically as a function in a free-fall, gravity-fed reactor. About 100g of the feed was then loaded into the gasifier applying "drop chute method" with the different mixture ratio of SP at 0, 25, 50, 75, 100% w/w. The electrical downdraft gasifier was heated with a WATLOW 240 V, 1300 W ceramic-embedded radiant tube heater with a maximum heating temperature of 1000 °C on continuous duty. Furthermore, the operating temperature varying from 650 °C to 850 °C was measured by an external PID controller coupled with a K-type thermocouple mounted on the gasifier reactor. Meanwhile, a stainless steel grate was held at the center inside the gasifier acted as the feedstock holder and also as the reactor bed where the thermal conversions took place. Air as an oxidizing agent was distributed in the gasifier by the compressed air through a 5 mm welded connection situated slightly below the top of the gasifier and controlled by a rotameter. The equivalence ratio of air fixed at 0.20, 0.25 and 0.30 was varied using the airflow rate from 2 L/min - 4L/min. The gasifier has two threaded openings at the top and bottom purposely for the feedstock loading and ash removal for cleaning access, respectively. Meanwhile, gases flowed towards the bottom of the reactor, certifying a downdraft fixed bed configuration [17]. The gases were then flowed to a gas conditioning unit before entering the online gas analyzer for gas composition measurement.



Figure 3. Schematic diagram of laboratory scale electrical downdraft gasifier used for the model validation.

The developed simulation model for co-gasification of CL and SP was used to perform the sensitivity analysis. The effect of the sawdust pellet (SP) blending ratio, gasification temperature and air equivalence ratio (ER) on each syngas composition, the calorific value of the syngas (CV_{syngas}), syngas yield (Y_{syngas}) and gasification efficiency (η GE) were investigated. The calorific value of the syngas (CV_{syngas}) was calculated as it is important output parameter that defines the quality of syngas produced from gasification in terms of energy content per unit volume or mass. The calorific value of the syngas (CV_{syngas}) was calculated by taking into account the volume percentage of combustible gas components in the syngas (CO, H₂ and CH₄) produced from the co-gasification experiment with their specific calorific value obtained from the US National Renewable Energy Laboratory (NREL) in the unit of MJ/Nm³ as per standard value [18]. The equation was expressed in *CVsyngas*=(*V_{CO}* × 12.63) + (*V_{CH4}* × 39.82) + (*V_{H2}* × 12.74)).

$$CV_{syngas} = (V_{C0} \times 12.63) + (V_{CH_4} \times 39.82) + (V_{H_2} \times 12.74)$$
(1)

Where CV_{syngas} is calorific value of the syngas in the unit of MJ/Nm³ and V is volumetric percentage for each of CO, CH₄ and H₂ obtained from online gas analyzer measurements (%). Meanwhile, the syngas yield (Y_{syngas}) in the unit for each experiment is taken into account the volume of syngas produced per unit mass of feedstock consumed in gasifier by considering the nitrogen balance method that has been proposed and applies by several authors [19]. It was applied by taking into account the continuous exposures of the high temperatures as well as the tar depositions in the measuring equipment cause the inaccuracy of the reading. The calculated value was given in Equation (2).

$$Y_{syngas} = \frac{Q_a \times 79\%}{m_{feed} \times N_2} \tag{2}$$

Where Y_{syngas} described as the syngas yield (Nm³/kg), Q_a is volume flow rate of air (Nm³/h), m_{feed} is mass flow rate of the feedstock in the gasifier system (kg/h) and N₂ % is refer to volumetric percentage of N₂ in the dry fuel gas. Furthermore, the gasification efficiency (η GE) can be calculated either from the cold gas efficiency or hot gas efficiency [20]. It is possible to define the cold gas efficiency as the ratio between the chemical energy leaving the system associated with the cold and tar-free syngas and the chemical energy energy entering the system related to the biomass [21]. Thus, the gasification efficiency was calculated by considering the specific gas production and the energy content of the biomass. The gasification efficiency (η GE) was calculated using Equation (3)

$$\eta GE = \frac{CV_{syngas} \times Y_{syngas}}{CV_{feed}} x \ 100 \tag{3}.$$

Where η GE is refer to gasification efficiency (%); CV_{syngas} and CV_{feed} is the calorific value of the syngas and feed respectively in the unit of MJ/kg. Meanwhile Y_{syngas} described as syngas yield (Nm³/kg). The comparison on the predicted data from the simulation model with experimental for the cogasification of CL and SP were discussed on the gasification performance in term of CV_{syngas}, Y_{syngas} and η GE. In additional, the root mean square error (RMSE) was calculated using Equation. (4) for each gasification performance at different gasification conditions to measure the error between simulation and experimental.

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n} (P_i - O_i)^2}{n}}$$
(4).

Where P, O and n refer to predicted value, observed value and number of dataset respectively.

3. Results and Discussions

A sensitivity analysis was performed in the GASIFIER block by varying the gasification temperature and airflow parameter at different sawdust pellet blending ratio. This was to investigate the effect of sawdust pellet blending ratio, gasification temperature and air equivalence ratio on the gasification performance. In ASPEN Plus, sensitivity tool was used to determine the gasification performance on the varying input parameter. Table 3 shows the input parameters of the temperature and airflow applied in the model.

Variable	Туре	Block/stream	Variable	Unit	Limits	Increment
Temperature	Block-var	GASIFIER	TEMP	°C	600-1000	50
Air flow	Stream-var	AIR	MASS-FLOW	kg/hr	0.1-0.4	0.025

Table 3. Range of input parameter for operational model

3.1. Effect of sawdust pellet blending ratio

Figures 4 (a), 4 (b) and 4 (c) present the effect of the sawdust pellet at blending ratio of 0, 25, 50, 75, 100% w/w on the CV_{syngas}, Y_{syngas} and η GE, respectively. The gasification temperature and the ER_{air} was fixed at 750 °C and 0.25. It can be seen that all the gasification performance increase with the increasing of the sawdust pellet blending ratio from 0 to 50%. The range of the CV_{syngas}, Y_{syngas} and η GE calculated were 3.00 - 6.00 MJ/Nm³, 1.00-2.00 Nm³/kg and 25% - 37%, respectively. It had been discovered that the maximum value of the CV_{syngas} at 5.78 MJ/Nm³, Y_{syngas} at 2.00 Nm³/kg and η GE at 37% were obtained from the simulation result that occur at 50% of the sawdust pellet blending ratio. However, as the amount of the sawdust pellet blending ratio increase to 75%, all of the gasification performance was dropped down averagely 30%. A similar trend had been found out by Seo et al. [22] that denoted the increasing of the Y_{syngas} at all temperature together with an increase in biomass ratio is due to the transfer

of hydrogen radicals in biomass to coal that resulted in higher decomposition of coal. It is noted that the suggested minimum blend 40% pine chips to 60% Sabero refuse coal by Pan et al. [23] with the value at 1.78 Nm^3/kg were quite similar to those for the highest yield of the syngas obtained from this study when assessing influence of the biomass blending ratio on the Y_{syngas} . In term of the RMSE value, both of the CV_{syngas} and Y_{syngas} are in the range of the 0 to 1.60 that is relatively low and generally well satisfactory with the experimental result. Hence, this denoted that the purpose model was validated and reliable. In contrast, the RMSE value of the η GE was in the range of the 0 to 21, in which the highest was recorded at 50% of the sawdust pellet blending ratio. This deviation might be due to the equilibrium condition that was applying in the gasification model that eliminated insignificant reaction between the coal and biomass [24].





Figure 4. Effect of the sawdust pellet blending ratio with calculated RMSE value on (a) CV_{syngas} (b) Y_{syngas} and (c) η GE at gasification temperature and E_{air} fixed at 750 °C and 0.25.

3.2. Effect of gasification temperature

The influence of the gasification temperature from 650 to 850 °C on various sawdust pellet blending ratio with the ER_{air} fixed at 0.25 on the gasification performance is illustrated in Figures 5 (a), 5 (c) and 5 (e) show the CV_{syngas}, Y_{syngas} and ŋGE as a function of gasification temperature, respectively. Meanwhile, the RMSE value for every gasification performance in term of CV_{syngas}, Y_{syngas} and ŋGE are illustrated in Figures 5 (b), 5 (d) and 5 (f), respectively. Altogether, it can be seen that the gasification temperature at the various sawdust pellet blending ratio exhibits an increase for all the performance parameters. The range of the CV_{syngas} was from 2.00 to 6.00 MJ/Nm³, and Y_{syngas} was ranged from 1.00 to 2.00 Nm³/kg. Furthermore, nGE was ranged from 18% to 37%. The maximum of each of the gasification performance occurs at 50% of the sawdust pellet blending ratio. It can be concluded that the optimum blending ratio for the sawdust pellet with coal was at 50%. A study conducted by Masnadi et al. [25] assesses that the increased of the CV_{syngas} is associated with higher gasification temperature resulted in the endothermic gasification reactions [26]. Complementary to this higher gasification temperature, more heat losses of the system and eventually improved the gasification process on the syngas production. Meanwhile, increasing of the gasification temperature enhance the release of gaseous product from the pyrolysis, steam reforming, gasification and cracking reactions inside the gasifier and contribute to the high total amount of Y_{syngas} [27]. These results were also attributed by several researchers that state the influence of temperature on Y_{syngas} in co-gasification [28]. Considering rising of the gasification temperature improved the endothermic char reactions in the gasifier, it can be concluded that the increase of the Y_{syngas} can be expected due to the increasing concentration of gaseous product [29]. It can be seen that the increase of ηGE as the gasification temperature increases is mainly due to the rise in CV_{syngas}. As previously mentioned, the lower RMSE value indicates the least error between simulation and experimental. It can be seen from the RMSE value for each the gasification performance parameter against the gasification temperature is lower than 20. Consequently, the model is suitable to serve as a preliminary for the co-gasification of coal with pellets.



Figure 5. Various gasification temperature of ER_{air} fixed at 0.25 on (a) CV_{syngas} (c) Y_{syngas} and (e) ŋGE with the respectively calculated RMSE (b), (d) and (f) on the different SP blending ratio.

3.3. Effect of air equivalence ratio (ER_{air})

 CV_{syngas} , Y_{syngas} and ηGE plot are presented in Figures 6 (a), (c) and (e), respectively for co-gasification of sawdust pellet at various blending ratio testing at gasification temperature fixed at 750 C. On the other hand, Figures 6 (b), (d) and (f) exhibited the calculated RMSEE value for each CV_{syngas} , Y_{syngas} and ηGE respectively. It can be seen that the CV_{syngas} and ηGE gradually decreased as the ER_{air} increased to 0.4. The CV_{syngas} and ηGE were ranged from 1.6 to 8.4 MJ/Nm³ and 14% to 51%, respectively. Both of

the highest of the CV_{syngas} were recorded at pure sawdust pellet achieved at 8.369 MJ/Nm³ and 51%, respectively. This can be predicted as the nature of the pellet form enhance the energy density per unit volume, uniformity and defined structure of fuels thus possess higher stability without depending on the critical variation of time [9]. In additional for others feed, increasing the ER_{air} contribute to the higher airflow rate resulted to the lower heating values for syngas and significantly reduced the gasification process efficiency [7,30]. This is believed to occur due to the ER_{air} is related to the airflow rate, therefore increasing of the airflow rate resulted in the shorter residence time of the feed to undergoes reactions (Basu, 2010; Yan et al., 2018). Inversely, increasing the ER_{air} value, the value of the Y_{sngas} also increased. The range of the Y_{syngas} at different sawdust pellet blending ratio is Upadhyay et al. [33] stated that the total Y_{syngas} is mainly associated with the fuel and air consumption rates. The study conducted on the cogasification of lignite and sawdust briquette was found that the higher gas yield was reached at 2.99 Nm³/kg that obtained at the high ER_{air} of 0.386. Commonly, it has been stated that for effective downdraft gasification, the ER is between 0.2-0.4 (Basu, 2010). For the RMSE value, as previously described, the RMSE value both for the CV_{syngas} and Y_{syngas} were lower ranged from 0 to 2.3. The RMSE value for ηGE was ranged from 0 to 32 that is quite high, which calculated at 50% of the sawdust pellet blending ratio. This might be due to the kinetic reaction that takes place in the gasifier during the experimental measurement.





Figure 6. Influence of ERair at the various sawdust pellet blending ratio from 0, 25, 50, 75, 100% w/w at gasification temperature 750 °C on the (a) CV_{syngas} (c) Y_{syngas} and (e) ηGE with the respectively calculated RMSE (b), (d) and (f).

4. Conclusions

Simulation modelling on the co-gasification of the coal and sawdust pellet was developed using the Aspen Plus software. The effect of the sawdust pellet blending ratio, gasification temperature and E_{air} on the gasification performance are investigated. The result shows that 50% of the sawdust pellet blending ratio in the co-gasification possess the maximum of the CV_{syngas}, Y_{syngas}, η GE at 5.84 MJ/Nm³, 2.00 Nm³/kg and 37%, respectively. Increasing of the gasification temperature are parallel increasing the gasification performance of the co-gasification. In additional, the sensitivity results indicate that the higher ER_{air} contribute to the lower value of the CV_{syngas} at 1.58 MJ/Nm³ and η GE at 14.52% that occur at 50% of the sawdust pellet blending ratio. Meanwhile, for the RMSE value; CV_{syngas} and Y_{syngas} shows relatively low value calculated at 0-2 and 0-1.5 indicated that the proposed model could be adopted to measure the gasification performance. In contrast, RMSE value on the η GE is calculated at 5-32 due to the equilibrium state assume in the model.

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