Performance Optimization of the Gasification Process by using Equilibrium Model and Dragonfly Algorithm

Adityabir Singh¹, Ranjan Das

Department of Mechanical Engineering, Indian Institute of Technology Ropar, Punjab, 140001, India ¹Corresponding author: E-mail: 2017mez0035@iitrpr.ac.in, Telephone: +91-9915372154

Abstract – The prediction of the working parameters is of importance for the optimum performance of the biomass gasification process. The gasification temperature, the initial moisture content of the biomass and the equivalence ratio are some of the main input parameters which decide the syngas composition and hence the gasification efficiency. Here, a modified equilibrium model based on a single global gasification reaction with equilibrium constants directly obtained from the available empirical relations is used to predict the syngas composition and the equivalence ratio at different values of moisture content and gasification temperature for two different biomasses (rubber wood and saw dust). The present model is relatively simpler than the available ones and is validated against both experimental and numerical data available for rubber wood and saw dust. Thereafter, the present modified model is used to study the variation in syngas composition, equivalence ratio, lower heating value of syngas and coldgas efficiency for different input values of gasification temperature and moisture content. Subsequently, an optimization problem is formulated by taking the ratio of equivalence ratio to the lower heating value of syngas as the objective function. The dragonfly algorithm is used for the optimization of the gasification temperatures varying in the range 800 °C to 1000 °C. The optimization results show that the maximum possible efficiency for rubber wood is 79.85% for 0.374 equivalence ratio and the same for saw dust is 85.00% for 0.302 equivalence ratio corresponding to the lowest gasification temperature and moisture content.

Keywords: gasification temperature; moisture content; equivalence ratio; lower heating value of syngas; coldgas efficiency; equilibrium model; dragonfly algorithm

1. Introduction

The growing demand of energy consumption attracts considerable attention of many researchers towards the optimization study of gasification process for various biomasses. For this purpose, many modelling schemes (equilibrium modelling, kinetic modelling, computational fluid dynamics modelling, modelling through artificial neural network and modelling using ASPEN Plus software) have been developed by various researchers for different types of gasifiers, as reported by Patra and Sheth [1]. These schemes enable to simulate the gasification process for a particular type of biomass under varying input parameters.

For modelling the gasification process in downdraft gasifiers under equilibrium conditions, Chern et al. [2] proposed a model to predict the gasification temperature ($T_{gasification}$) and syngas composition (SC) for different air to feed mass ratio and moisture to feed mass ratio. Zainal et al. [3] predicted the variation of the SC and the corresponding value of the equivalence ratio (ϕ) for any input value of $T_{gasification}$ and moisture content (MC). Mountouris et al. [4] improved the model reported by Zainal et al. [3] by correcting the method of calculating enthalpy formation of the woody biomass. Jarungthammachote and Dutta [5] also improved the model of Zainal et al. [3] by multiplying coefficients calculated from the average value of ratios of methane and carbon monoxide with equilibrium constants. Thus, they predicted the SC and ϕ quite close to the experimental values under varying $T_{explication}$ and the MC. Vaezi et al. [6] modified the model of Jarungthammachote and Dutta [5] to calculate the carbon/hydrogen ratio and oxygen content (characteristics of biomass) for a particular application defined by the syngas properties. Sreejith et al. [7] performed a parametric study through Gibbs energy minimization approach in conjunction with the simulated annealing method by varying $T_{gasification}$ and pressure of the gasification process. Sharma and Sheth [8] incorporated char into the global gasification reaction proposed by Zainal et al. [3] and evaluated the SC and $T_{gasification}$ by varying the MC and ϕ . Shayan et al. [9] considered the oxides of nitrogen and sulphur in the global gasification reactions and then evaluated the hydrogen production by varying the $T_{gasification}$ and MC. Tauqir et al. [10] modelled the gasification process through equilibrium approach, using ASPEN Plus software and studied the effect of $T_{gasification}$, MC and ϕ on the SC, lower heating value of the syngas (LHV_{syngas}) along with hot gas efficiency and cold gas efficiency ($\eta_{coldgas}$). For wood and agricultural based biomasses, Ayub *et al.* [11] improved the equilibrium model by adding correction factors based on the experimental data into the design equations. Caglar et al. [12] calculated the variation of the production of syngas yield, hydrogen production, methane production, carbon dioxide emission and gasification efficiencies with respect to $T_{gasification}$ and different gasifying agents. Yan et al. [13] clubbed the gasification equilibrium model with the artificial neural network model, and later performed the analysis for different physical dimensions of the gasifier, $T_{gasification}$, MC and ϕ .

From the above analysis, it is found that to the best of the authors' knowledge there is no study that either provides the optimum values MC and ϕ , when gasification is performed at some fixed value the $T_{gasification}$ or that determines the optimum values of $T_{gasification}$ and ϕ , when biomass with a fixed MC is used. To address this gap, in the present work, an optimization problem is defined, which provides the optimum values of MC and ϕ for a fixed $T_{gasification}$, and the optimum values of $T_{gasification}$ and ϕ for a fixed MC, such that the LHV_{syngas} and $\eta_{coldgas}$ attain their maximum possible values. Here, the model proposed by Jarungthammachote and Dutta [5] is modified by combining the empirical relations of the equilibrium constants reported in the study of Zainal et al. [3] that provides a simpler approach without any considerable compromise in the accuracy of the output.

2. Gasification modelling and its validation

In the proposed simulation, the equilibrium model proposed by Jarungthammachote and Dutta [5] is modified. This is done by defining the chemical equilibrium through equilibrium based on the general equations provided by Zainal et al. [3] instead of standard Gibbs function as adopted by Jarungthammachote and Dutta [5]. The general equations are discrete functions of $T_{gasification}$. The present model is capable to predict the SC and ϕ corresponding to maximum syngas yield for any input value of $T_{gasification}$ and MC.

2.1. Equilibrium model

The gasification of 1 kmol of dry biomass ($CH_{\alpha}O_{\beta}N_{\delta}$) with air (as a gasification agent) is represented by a single chemical equation written as,

Gasification reaction [5],

$$CH_{\alpha}O_{\beta}N_{\delta} + mH_{2}O_{(moisture)} + n(O_{2} + 3.76N_{2}) \rightarrow f_{1}H_{2} + f_{2}CO + f_{3}CO_{2} + f_{4}H_{2}O_{(vapor)} + f_{5}CH_{4} + \left(\frac{\delta}{2} + 3.76n\right)N_{2}$$
(1)

where, α , β and δ are the atomic ratios of hydrogen, oxygen and nitrogen with respect to carbon atom. The symbol m represents the amount of moisture (kmol/kmol_{biomass}) and n represents the oxygen (kmol/kmol_{biomass}) supplied for gasification. Further, the symbols f_1 , f_2 , f_3 , f_4 and f_5 represent the SC (kmol/kmol_{biomass}) produced after the gasification process. The Eq. (1) has six unknowns $(n, f_1, f_2, f_3, f_4 \text{ and } f_5)$, which are to be calculated for the given $T_{gasification}$ and MC in the biomass. The value of m can be calculated from the input value of MC (in percentage), by following the work of Zainal et al. [3]. Next, the molar, enthalpy and equilibrium balance is performed to obtain six equations for calculating the unknowns. The global gasification equation, Eq. (1) is used for the molar and enthalpy balances,

Molar balance [5],

Carbon balance:
$$1 = f_2 + f_3 + f_5$$
 (2)

$$Iydrogen balance: 2m + \alpha = 2f_1 + 2f_4 + 4f_5$$
(3)

Hydrogen balance :
$$2m + \alpha = 2f_1 + 2f_4 + 4f_5$$
 (3)
Oxygen balance : $m + 2n + \beta = f_2 + 2f_3 + f_4$ (4)

Enthalpy balance [5],

$$H_{f,\text{biomass}}^{o} + m \Big[H_{f,\text{H}_{2}\text{O}(\text{liq.})}^{o} + H_{\text{vaporization}} \Big] + n H_{f,\text{O}_{2}}^{o} + 3.76n H_{f,\text{N}_{2}}^{o} = f_{I} \Big[H_{f,\text{H}_{2}}^{o} + c_{P,\text{H}_{2}} \Big(T_{gasification} - T_{o} \Big) \Big] + f_{2} \Big[H_{f,\text{CO}}^{o} + c_{P,\text{CO}} \Big(T_{gasification} - T_{o} \Big) \Big] + f_{3} \Big[H_{f,\text{CO}_{2}}^{o} + c_{P,\text{CO}_{2}} \Big(T_{gasification} - T_{o} \Big) \Big] + f_{4} \Big[H_{f,\text{H}_{2}\text{O}_{(\text{vapor})}}^{o} + c_{P,\text{H}_{2}\text{O}_{(\text{vapor})}} \Big(T_{gasification} - T_{o} \Big) \Big] + f_{5} \Big[H_{f,\text{CH}_{4}}^{o} + c_{P,\text{CH}_{4}} \Big(T_{gasification} - T_{o} \Big) \Big] + \Big(\frac{\delta}{2} + 3.76n \Big) \Big[H_{f,\text{N}_{2}}^{o} + c_{P,\text{N}_{2}} \Big(T_{gasification} - T_{o} \Big) \Big] \Big]$$
(5)

where, H_{f}^{o} represents the enthalpy of formation (in kJ/kmol) at ambient conditions (25 °C and 1 atm) for the reactants and products. H_{vaporization} is the enthalpy of vaporization of moisture in kJ/kmol. Since the product is at higher temperature equal to $T_{gasification}$, therefore, the product of specific heat at constant pressure, c_p in kJ/(kmol.K) and the temperature difference is added in H_f^o for each chemical species on the product side. For the equilibrium balance, water-gas shift reaction and methane formation reaction are considered [5]. The chemical equations of both the reactions are given below,

Water-gas shift reaction [5],

$$CO + H_2O \rightarrow CO_2 + H_2 \tag{6}$$

Methane formation reaction [5],

$$C + 2H_2 \rightarrow CH_4 \tag{7}$$

The equilibrium constant from the water-gas shift reaction and methane formation reaction are written below, Equilibrium constant for water-gas shift reaction [5],

$$\kappa_1 = \frac{f_3 f_1}{f_2 f_4} \tag{8}$$

Equilibrium constant for methane formation reaction [5],

$$\kappa_2 = \frac{f_5 f_{total}}{\left(f_1\right)^2} \tag{9}$$

where, f_{total} represents total molar fraction of the syngas produced after the gasification. The values of κ_1 and κ_2 which vary with $T_{gasification}$ are calculated from the direct expressions available in Zainal *et al.* [3]. Eqs. (2-5, 8 and 9) are solved to predict the values of n, f_1 , f_2 , f_3 , f_4 and f_5 , at the given $T_{gasification}$ and *MC*. The value of ϕ is then calculated from the value of n by following the work of Li *et al.* [14].

2.2. Validation of the proposed model

To validate the present model, a comparison is done with the work of Jayah *et al.* [15], Jarungthammachote and Dutta [5] and Altafini *et al.* [16] by setting the values of $T_{gasification}$ and *MC* equal to those reported in the concerned works. The composition of nitrogen written as ($\delta/2+3.76n$) in Eq. (1)) is referred as $f_6 = (\delta/2+3.76n)$] in Table 1. The composition of syngas (f_1, f_2, f_3, f_5 and f_6) is represented in molar percentage for easy comparison with the literature as shown in Table 1.

Tuble 1. Vullauton of the present model with the numerical and experimental data.									
	Rubber wood			Saw dust					
Parameters	Experimental	Equilibrium	Present	Experimental	Cycle-Tempo	Equilibrium	Present		
	data ^(a)	model ^(b)	model	data ^(c)	model ^(c)	model ^(b)	model		
Input parameters									
T _{gasification} (°C)	827.00	827.00	827.00	800.00	800.00	800.00	800.00		
MC (%)	16.00	16.00	16.00	10.00	10.00	10.00	10.00		
Output parameters									
f_l (mol. %)	17.00	16.81	17.77	14.00	21.40	18.24	19.88		
f_2 (mol. %)	18.40	17.86	18.80	20.14	23.00	23.34	25.68		
f_3 (mol. %)	10.60	12.10	11.80	12.06	9.74	9.82	8.88		
$f_5 ({\rm mol.}\%)$	1.30	1.05	1.16	2.31	0.01	1.66	1.94		
$f_6 ({ m mol.}\%)$	52.70	52.18	50.47	50.79	45.31	46.93	46.61		

Table 1: Validation of the present model with the numerical and experimental data

Note: The superscripts represents data from (a) Jayah et al. [15], (b) Jarungthammachote and Dutta [5] and (c) Altafini et al. [16]

From Table 1, the predicted composition closely agrees with the experimental work of Jayah *et al.* [15], and is also found to predict better results when compared with the results of Cycle-Tempo model (particularly for f_5) used by Altafini *et al.* [16]. The present model predicted higher percentages of f_1 , f_2 , and f_5 , but lower percentages of f_3 and f_6 when compared with the results of Jarungthammachote and Dutta [5]. The results from the present model for rubber wood are compared in terms of root-mean-square error, which is, 1.20 against the experimental data of Jayah et al. [15], and 0.98 against the data of Jarungthammachote and Dutta model [5]. For saw dust, the error is 4.31 with respect to the experimental data of Altafini *et al.* [16], 1.77 against the data of cycle-tempo model and 1.36 when compared with Jarungthammachote and Dutta model [5].

2.3. Energy analysis

The LHV_{syngas} defines the energy output of the biomass gasifier. The predicted values of molar percentage of hydrogen, carbon monoxide and methane are mainly used for its calculation (in MJ/kmol_{biomass}), as shown below,

Syngas heating value [17],

$$LHV_{syngas} = 22.4 \Big[(f_1 / 100) LHV_{H_2} + (f_2 / 100) LHV_{CO} + (f_5 / 100) LHV_{CH_4} \Big] y$$
(10)

where, the *LHV* is the lower heating value of hydrogen, carbon monoxide and methane (in MJ/m³), and y represents the kmol of syngas produced per kmol of biomass. The $\eta_{coldgas}$ of the gasification of the biomass is expressed as shown below,

Gasification efficiency [17],

$$\eta_{coldgas} = \frac{LHV_{syngas}}{LHV_{biomass}}$$
(11)

where, the *LHV*_{biomass} is the lower heating value of biomass in MJ/kmol_{biomass}.

3. Results

The validated equilibrium model is used to study the effect of MC and $T_{gasification}$ on the SC for rubber wood and saw dust. The characteristic properties of the rubber wood is taken from Jayah *et al.* [15] and that for saw dust is taken from Altafini *et al.* [16].



To study the individual effect *MC* and $T_{gasification}$ on the *SC*, firstly it is assumed that the gasification is performed at 800 °C [15] and the *MC* in both the biomasses is varied from 5 % to 25 % [18] as shown in Fig. 1. There is an enhancement in the percentage of f_1 (17.00% to 18.88% for rubber wood and 19.17 % to 21.74 % for saw dust) and f_3 (9.98 % to 13.83 % for rubber wood, and 7.62% to 12.63% for saw dust). This is due to favourable conditions for water-gas shift reaction mentioned in Eq. (6), which consumes carbon monoxide (reason for decrease in f_2 from 21.68 % to 16.23 % for rubber wood and 27.41 % to 20.36 % for saw dust) with moisture to produce hydrogen and carbon dioxide. Similarly, the slight increase in f_5 (1.41 % to 1.62 % for rubber wood and 1.84 % to 2.20 % for saw dust) is due to the presence of more hydrogen for methane formation reaction given in Eq. (7). The percentage of f_6 almost remains constant (49.92 % to 49.44 % for rubber wood and 43.96 % to 43.06 % for saw dust).

In the present work, $T_{gasification}$ is assumed to vary from 800 °C to 1000 °C [10] at 15 % *MC* [10] as shown in Fig. 2. The decrease in f_1 (18.03 % to 14.34 % for rubber wood, and 20.56% to 17.21% for saw dust), f_3 (11.91% to 10.84% for rubber wood, and 10.14 % to 9.19 % for saw dust) and f_5 (1.54% to 0.19% for rubber wood, and 2.05% to 0.28% for saw dust) is due to the exothermic nature of both water-gas and methane formation reaction. The increase in $T_{gasification}$ shifts both the reactions expressed by Eqs. (6, 7) in the reverse direction [10]. This results in the decrease in the percentage of f_1 , f_3 and f_5 . The percentage of f_2 almost remains constant (19.00% to 18.61% for rubber wood, and 23.93% to 23.02% for saw dust), while the value of f_6 increases (49.53% to 56.02% for rubber wood, and 43.33% to 50.31% for saw dust) due to increase in the value of n (kmol of oxygen) with increase in $T_{gasification}$.





Next, for a fixed $T_{gasification} \approx 800$ °C, the effect of variation in the *MC* on ϕ , *LHV*_{syngas} and $\eta_{coldgas}$ is studied in Fig. 3. It is seen that the value of ϕ increases (0.374 to 0.387 for rubber wood and 0.302 to 0.310 for saw dust) with the *MC*. This is because the moisture in the biomass requires heat for its vaporization, which lowers $T_{gasification}$. So, the value of ϕ must increase (means more air for gasification) to maintain constant temperature during gasification. The decrease in the *LHV*_{syngas} (344.05 MJ/kmol_{biomass} to 330.15 MJ/kmol_{biomass} for rubber wood, and 376.08 MJ/kmol_{biomass} to 363.20 MJ/kmol_{biomass} for saw dust) is due to the more reduction in the percentage of f_2 , as compared to the increase in the percentage of f_1 and f_5 [please refer, Eq. (10)]. Due to the decrease in *LHV*_{syngas}, the value of $\eta_{coldgas}$ also decreases (79.85% to 76.63% for rubber wood, and 85.00% to 82.09% for saw dust) as seen from Eq. (11).







Fig. 4: The effect of $T_{gasification}$ on the ϕ , LHV_{syngas} and $\eta_{coldgas}$ for (a) rubber wood and (b) saw dust.

Similarly, for $MC \approx 15\%$, the study of variation in $T_{gasification}$ on ϕ , LHV_{syngas} and $\eta_{coldgas}$ is performed in Fig. 4. Since more air must be supplied to increase the value of $T_{gasification}$ from 800 °C to 1000 °C, which leads to raise the value of ϕ (0.379 to 0.469 for rubber wood, and 0.304 to 0.393 for saw dust). Further, the decrease in the LHV_{syngas} (338.11 MJ/kmol_{biomass} to 299.90MJ/kmol_{biomass} for rubber wood, and 370.64 MJ/kmol_{biomass} to 335.58 MJ/kmol_{biomass} for saw dust) can be explained in terms of reduction in the percentage of f_1 and f_5 (please refer Eq. 10) with rise in $T_{gasification}$. As evident from Eq. (11), the decrease in LHV_{syngas} also leads to decrease in $\eta_{coldgas}$ (78.48% to 69.61% for rubber wood, and 83.77% to 75.85% for saw dust) of the biomass gasification.

To formulate an optimization problem from the above analysis, it is evident that the optimum conditions lie at that point where ϕ is at its minimum and *LHV*_{syngas} is at its maximum. This can be explained in terms of the amount of air intake, which dilutes the *SC* (since rise in ϕ also increases the amount of nitrogen in the syngas) and hence reduces the value of *LHV*_{syngas}. So, the objective function (*fobj*) to be minimized can be taken as ϕ/LHV_{syngas} . Here, the dragonfly algorithm, developed by Mirjalili [19], is used as an optimization tool and its search area is defined by the range of variation in $T_{gasification}$ and *MC*. It is based on the behaviour characteristics (hunting and migration) of the dragonflies within the population, as explained in the published work [20, 21]. In order to avoid local optimum solution, the dragonfly algorithm uses Lévy flight distribution to maintain randomness in the swarming pattern of the dragonflies. This enables the algorithm to converge faster and closely leads to global optimum solution. Both population size (number of dragonflies) and the number of iterations (number of times the optimization process is repeated) is taken 50.



Fig. 5: Variation of the *fobj* and *MC* with iterations for (a) rubber wood and (b) saw dust, and variation of the *fobj* and $T_{gasification}$ with iterations for (c) rubber wood and (d) saw dust

The convergence of the problem is assessed in Fig. 5 for the biomasses studied. Fig. 5 (a, b) represents the variation of *fobj* and *MC* (ranging between 5% to 25%) with iterations for different $T_{gasification}$ (800 °C, 850 °C and 900 °C), and Fig. 5 (c, d) signifies the variation of *fobj* and $T_{gasification}$ (ranging between 800 °C to 1000 °C) for different *MC* (5%, 10% and 15%). It is clear that the assumed population and iterations are sufficient for the convergence of the optimization problem.

Table 2 presents the optimized results at different $T_{gasification}$ for both biomasses, when *MC* ranges from 5% to 25%. Here, maximum and minimum are set the same for one complete optimization. It is seen that the optimum value of *MC* for any fixed $T_{gasification}$ is the minimum value of the search domain for all cases, and the corresponding optimum (minimum possible) value of ϕ is also shown. So, if the gasification is performed at fixed $T_{gasification}$ (≈ 800 °C), then the *MC* in the biomass (e.g. rubber wood) should be 5% and ϕ should be 0.374, to obtain maximum possible *LHV*_{syngas} (344.05 MJ/kmol_{biomass}) and $\eta_{coldgas}$ (79.85%). Similarly, Table 3 presents the optimization for different *MC* (the maximum and the minimum search limits are kept the same), when the search area of $T_{gasification}$ ranges from 800 °C to 1000 °C. Clearly, the optimum $T_{gasification}$ remains the same for all cases and is the minimum value of the search space. So, if the biomass (rubber wood) with $MC \approx 10\%$ is to be used during gasification, then $T_{gasification}$ and ϕ should be 800 °C and 0.376, to obtain maximum possible *LHV*_{syngas} (341.29 MJ/kmol_{biomass}) and $\eta_{coldgas}$ (79.21%).

	Optimized results						
$T_{gasification}$ (°C)	fobj	MC	ϕ	LHV _{syngas}	$\eta_{coldgas}$		
	(MJ/kmolbiomass)-1	(%)	(-)	(MJ/kmol _{biomass})	(%)		
For rubber wood							
800	0.001088	5	0.374	344.05	79.85		
850	0.001189	5	0.398	335.03	77.76		
900	0.001287	5	0.420	326.09	75.68		
950	0.001384	5	0.439	317.15	73.61		
1000	0.001484	5	0.457	308.18	71.53		
For saw dust							
800	0.000803	5	0.302	376.08	85.00		
850	0.000885	5	0.326	367.85	83.14		
900	0.000962	5	0.346	359.69	81.30		
950	0.001037	5	0.365	351.54	79.46		
1000	0.001113	5	0.382	343.35	77.61		

Table 2: Optimization performed by using ϕ/LHV_{syngas} as *fobj* for different fixed values of $T_{gasification}$

Table 3: Optimization performed by using ϕ/LHV_{syngas} as *fobj* for different fixed values of *MC*.

	Optimized results						
<i>MC</i> (%)	fobj	$T_{gasification}$	ϕ	LHV _{syngas}	$\eta_{coldgas}$		
	(MJ/kmol _{biomass}) ⁻¹	(°C)	(-)	(MJ/kmol _{biomass})	(%)		
For rubber wood							
5	0.001088	800	0.374	344.05	79.85		
10	0.001102	800	0.376	341.29	79.21		
15	0.001120	800	0.379	338.11	78.47		
20	0.001143	800	0.382	334.44	77.62		
25	0.001173	800	0.387	330.15	76.63		
For saw dust							
5	0.000803	800	0.302	376.08	85.00		
10	0.000810	800	0.303	373.56	84.43		
15	0.000820	800	0.304	370.64	83.77		
20	0.000834	800	0.306	367.22	83.00		
25	0.000853	800	0.310	363.20	82.09		

4. Conclusions

This paper demonstrates the role of $T_{gasification}$, MC and ϕ on the gasification performance through a modified equilibrium model, which incorporates direct empirical relations of equilibrium constants to predict the *SC*. The increase in the *MC* is found to improve the *SC*, but it also consumes more heat from the gasification reactions for its vaporization and hence requires more ϕ to carry out the gasification. This leads to dilution of the *SC* and hence reduces the $\eta_{coldgas}$. Similarly, the increase in the $T_{gasification}$ requires more ϕ , which adds more nitrogen in the system and hence also dilutes the *SC*. In order to improve the gasification performance, an optimization problem is framed which tends to maximize the *LHV*_{syngas} at the minimum possible value of ϕ . When optimized for fixed $T_{gasification}$, the *MC* in the biomass reduces to the minimum possible value, which leads to lesser consumption of heat from the gasification reactions, and thus improves the $\eta_{coldgas}$ to

the maximum possible value. Similarly, for optimization at a fixed *MC*, the gasification process is found to be optimum at the lowest possible value of $T_{gasification}$, as it accelerates both the water-gas and methane formation reactions in the forward direction. This in turn also lowers the value of ϕ . The present analysis provides useful guidelines towards the selection of working parameters at different gasification conditions in an optimized manner.

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