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Study on Predicting the Gasification Process of Acacia Wood on a Downdraft Gasifier: Using the Non-stoichiometric Equilibrium Model

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ABSTRACT

This study presents a prediction of acacia wood of Vietnam gasification in a downdraft gasifier based on the thermodynamic equilibrium model. Analytical solution for the mathematical model obtained by using an EES (Engineering Equation Solver) program. In the survey, moisture content per mole of biomass MC= 10 ÷ 30%, The ratio of the actual amount of oxygen used for gasification with the amount of oxygen for complete combustion of the biomass ER= 0.21 ÷ 0.4. Results indicated that the lower heating value of syngas decreases with increasing MC or ER. Thermal efficiency tends to increase with rising ER from 0.21 to 0.374, and it will decrease if ER continues to increase. The lower heating value of dry products from 4.51 to 6.51 MJ/nm^3, the heat efficiency from 49.62 to 75.53%. The carbon conversion factor tends to increase with an increase as MC or ER. The influence of MC on the carbon conversion factor is insignificant. The content of CO_2 and CH_4 increased, the content of CO decreased with increased MC or ER. The composition of H_2 increases as MC increases while the H_2 component increases slightly and then decreases with increasing ER.

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1. Introduction

Environmental pollution, climate change, and fossil fuel depletion are significant challenges facing humanity. Using renewable energy is a sustainable development direction in the future. Biomass is assessed to have great potential and low impact on the environment, and it can replace fossil fuels. Biomass energy can be converted to product by biological or thermochemical processes. Thermochemical conversion is in three forms: combustion, pyrolysis, and gasification. Gasification is a biomass conversion technology by partially oxidizing into a gaseous mixture. The conversion rates of this technology are evaluated to be higher than combustion and pyrolysis. Gasification is a favorable solution to reuse biomass solids. Gasification is a complex process and is affected by several parameters such as biomass composition, temperature gasification zone, gasifying agent, moisture of biomass, etc.

Various gasification models have been considered, such as kinetic models, computational fluid dynamics models, and thermodynamic equilibrium models to predict the gasification process of biomass. The thermodynamic equilibrium model is widely used because of its simplicity and less computation time. There are two types of thermodynamic equilibrium models: the stoichiometric and non-stoichiometric models. The stoichiometric equilibrium model is built when considering chemical reactions reach equilibrium, and the equilibrium constants need to be determined to solve this model, while the non-stoichiometric model uses Gibbs free energy minimization to estimate the equilibrium constant [1]. The non-stoichiometric equilibrium model has been used in many studies such as Altafini et al. [2], Melgar et al. [3], Haryanto et al. [4], Buragohain et al. [5]. The non-stoichiometric equilibrium model incorporating the carbon conversion factor has been considered in some studies such as Azzone et al. [6], Uzair Ayub [1]. Studies show that this model use has predictions quite suitable to the experiments of some types of biomass.

In the gasification process, the gasification temperature and product composition are highly dependent on the amount of oxygen supplied. It is a function of the amount of oxygen supplied to the gasifier, and this oxygen supply is usually expressed as an equivalence ratio, MR- the ratio of the actual amount of oxygen used for gasification with the amount of oxygen for complete combustion of the biomass. If little oxygen is used, some Char is not converted, while if much oxygen is used, more combustion occurs, and the temperature increases significantly [7]. Previous studies showed that ER=0.25 is the mode in which the efficiency of wood gasification can reach the maximum [7]. Therefore, an equivalence ratio near ER= 0.25 is preferred when operating the gasifier. In the equilibrium model incorporating the carbon conversion factor, the carbon conversion factor is a simple correlation with the ER by the empirical, with ER in the range ER = 0.21÷0.4 [6, 8].

Vietnam has a very large acacia growing area with millions of hectares of acacia. Therefore, acacia wood has great potential for exploitation and gasification to produce electricity or supply industrial processes. It is necessary to study the gasification process of acacia wood. In this study, a non-stoichiometric equilibrium model incorporating the carbon conversion factor was used to forerun the trend of the gas composition in the finished gas, thermal efficiency, and lower heating value of the dry product when gasifying acacia wood on the downdraft gasifier. Previous studies considered ER and gasification temperature as independent variables to investigate. This study will predict the gasification process from the point of view of gasification temperature as the dependent variable of ER to investigate the impact on output parameters and assess the suitability of the model with experimental results previously published. Furthermore, there will be an evaluation of the application of predictive models in research and teaching on biomass gasification. This study will investigate the predictions in scope ER=0.21÷0.4, and initial wood moisture MC=10÷30%.

2. Biomass gasification model

The main reactions in gasification include [9]:

+ The reaction produces carbon monoxide and hydrogen: $C + H_2O \rightarrow CO + H_2$ (1)

+ The reaction produces metal: $C + 2H_2 \leftrightarrow CH_4$ (2)

+ The reaction produces carbon monoxide: $C + CO_2 \leftrightarrow 2CO$ (3)

+ The reaction produces carbon dioxide and hydrogen: $CO + H_2O \leftrightarrow CO_2 + H_2$ (4)

The equilibrium model of gasification is considered with the assumptions:

- Ignore mineral and nitrogen components in biomass.
- Tar and Ash are considered to be inert.
- The inlet temperature of the feedstock and the air is 25°C.
- The pressure of gasification is 101325 N/m^2.
- The gasification is considered adiabatic.

The gasification reaction inside the gasifier is considered as follow [10]:

$$CH_aO_b + mH_2O + nO_2 + 3.76nN_2 = (1-\alpha)C + x_aH_2 + x_bCO + x_cCO_2 + x_dH_2O + x_eCH_4 + 3.76nN_2 \quad (5)$$

where x_a, x_b, x_c, x_d, x_e, $(1-\alpha)$ are moles of components in the reaction. m and n are the molar of water and oxygen per mole of feedstock, respectively.

The carbon conversion factor can be determined as follows [6], [8].

$$\alpha = 0.32 + 0.84\left(1 - e^{-ER/0.229}\right),\ ER = 0.21 \div 0.4 \quad (6)$$

With *m* and *n* can be determined by the following equations [10]:

$$n = ER\left(1 + \frac{a}{4} - \frac{b}{2}\right) \quad (7)$$

$$m = \frac{MC(12 + a + 16b)}{18(1 - MC)} \quad (8)$$

where *ER* is an equivalence ratio- the ratio of the actual amount of oxygen used for gasification with the amount of oxygen for complete combustion of the biomass, *MC* is initial moisture content of feedstocks.

The balanced equation of the components in the reaction are determined:

+ For carbon: $x_b+x_c+x_e=\alpha$ (9)

+ For Hydrogen: $2m+a=2x_a+2x_d+4x_e$ (10)

+ For Oxygen: $m+b+2n=x_b+2x_c+x_d$ (11)

The equilibrium constant for methane formation [10]:

$$k_1=\frac{x_e.x_t}{x_a^2} \tag{12}$$

where $x_t=x_a+x_b+x_c+x_d+x_e$ (13)

The equilibrium constant for water–gas shift [10]:

$$k_2=\frac{x_a x_c}{x_b x_d} \tag{14}$$

The equilibrium constant k_1 and k_2 can be determined [11]:

$$\ln k_1=7082.842T^{-1}-6.567\ln\mathrm{T}+3.7335.10^{-3}T-3.61167.10^{-7}T^2+35050.T^{-2}+32.541 \tag{15}$$

$$\ln k_2=5878T^{-1}+1.86\ln\mathrm{T}-0.27.10^{-3}T-58200T^{-2}-18 \tag{16}$$

Heat balance equation for gasification (considered adiabatic) [11]:

$$\begin{aligned}&H_{biomass}+mH^o_{H_2O,l}+H_{vap}+n.H^o_{O_2}+3,76n.H^o_{N_2}=(1-\alpha)H^o_C+x_aH^o_{H_2}+x_bH^o_{CO}+x_cH^o_{CO_2}+x_dH^o_{H_2O,g}\\&+x_eH^o_{CH_4}+[(1-\alpha)c_{p,\mathrm{C}}+x_ac_{p,H_2}+x_bc_{p,co}+x_cc_{p,CO_2}+x_dc_{p,\mathrm{H_2O}}+x_ec_{p,\mathrm{CH_4}}+3,76nc_{p,\mathrm{N_2}}]\Delta T\end{aligned} \tag{17}$$

where $c_{p,i}$, H_i^o, $H_{biomass}$, $H^o_{H_2O,l}$, and H_{vap} are specific heat, heat formation, heat formation of biomass, heat formation of liquid water, and heat of vaporization of water, respectively.

The specific heat of the components is determined [11]:

$$c_p=R(A+BT_{am}+\frac{C}{3}(4T_{am}^2-T_1T_2)+\frac{D}{T_1T_2}) \tag{18}$$

where A, B, C, and D are constants for the components (see [11]), T_1, T_2, and R are the ambient temperature, gasification temperature, and universal gas constant, respectively.

The heat formation of biomass (CH_aO_b) is calculated as follows [11]:

$$H_{biomass}=H^o_{CO2}+\frac{a}{2}H^o_{H_2O}+LHV_{biomass} \tag{19}$$

The lower heating value ($LHV_{biomass}$) of the feedstocks can be estimated by [12]:

$$LHV_{biomass}=\left(0.0041868+0.00062802[O]\right)\left(7837.667[\mathrm{C}]+33888.889[H]-0.125[O]\right) \tag{20}$$

where [C], [H], [O], and [A] are the ultimate analysis of C, H, O, and Ash, respectively.

To evaluate the accuracy of the model, the root mean square (RMS) error was used [10]:

$$RMS=\sqrt{\frac{\sum(A_e-A_p)^2}{Y}} \tag{21}$$

where A_e, A_p, and Y are the result of experiment, result of predicted, and number of experiments performed, respectively.

The volume percent of the dry syngas is calculated as follows:

$$[V_i] = \frac{x_i}{\sum_{i=1}^{4} x_i} \tag{22}$$

where x_i are the moles of H_2, CO, CO_2, CH_4

Lower heating value (LHV_{gas}, MJ/Nm^3) of dry product is estimated [13]:

$$LHV_{gas} = 4.2(3[V_{CO}] + 2.57[V_{H2}] + 8.54[V_{CH4}]) \tag{23}$$

The heat efficiency of the gasifier (efficiency of cold gas) can be estimated as follows [10]:

$$\eta = \frac{22.4 x_{total}}{M_{bm}} \cdot \frac{LHV_{gas}}{LHV_{biomass}} \tag{24}$$

where M_{bm} is inlet mass of biomass, x_{total} is moles of the dry syngas

The sets of equations (6-24) were solved by the EES software (Engineering Equation Solver) to determine the variables in the 19 equations above. This program allows solving sets of equations, including linear and nonlinear equations, simply and quickly. The algorithm flowchart used to survey the parameters in this study is shown in Figure 1.

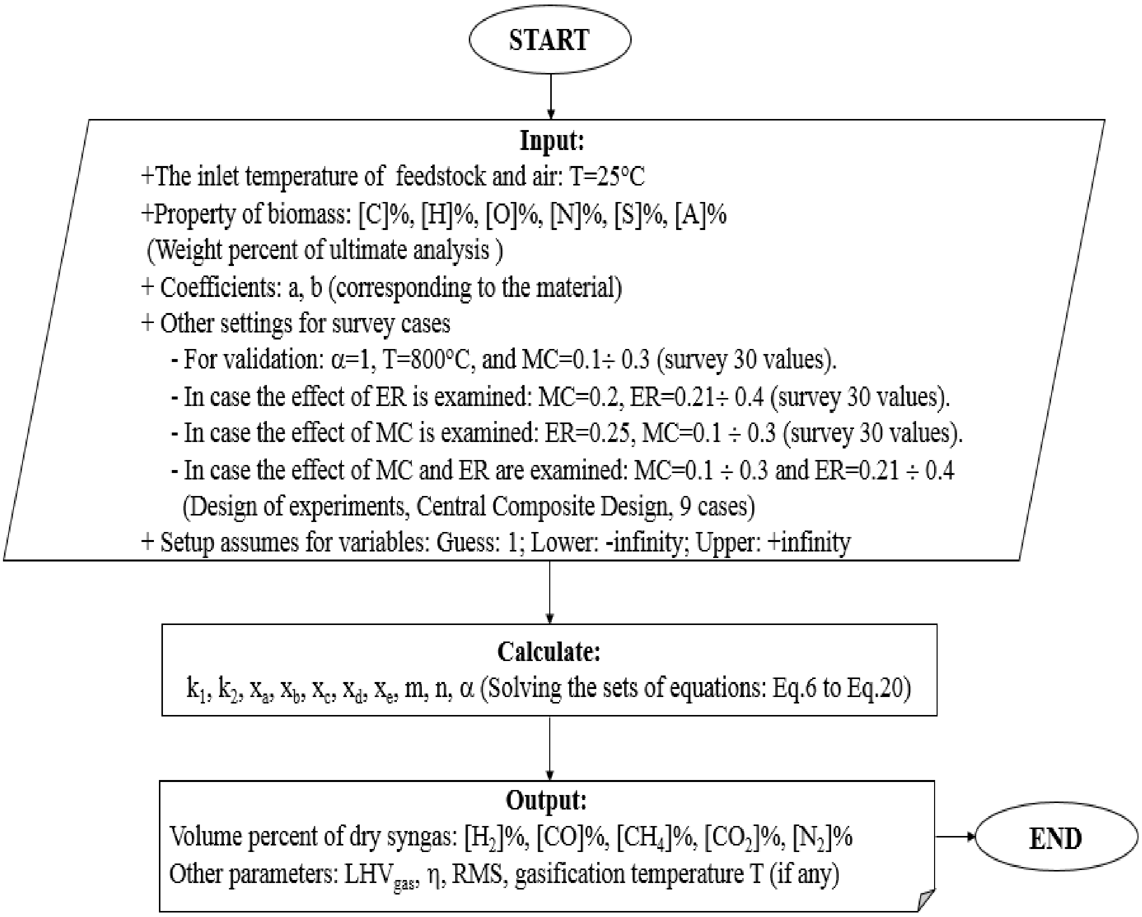


Figure 1. *Algorithm Flowchart to solve the problem*

The analysis for wood: [C] (50%), [H] (6%), [O] (44%), [N] (0%), [A] (0%), carbon conversion factor α=1 and the gasification temperature T=800°C was performed to verify the mathematical model. The results show that the volume percent of gases in the present study is in good agreement with published data [11] (Figure 2). Thus, the calculation program can be trusted to predict gasification for acacia wood.

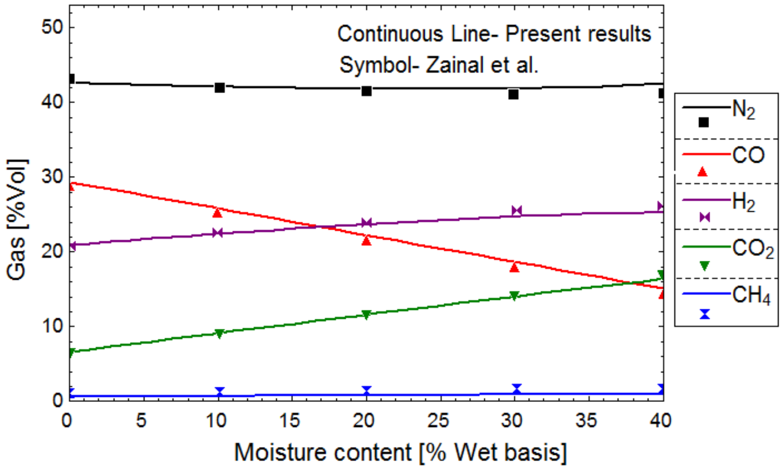


Figure 2. *Validation with published result [11]*

3. Results and Discussion

The gasification predictions in this study were performed for acacia wood with property parametric shown in Table 1. Table 2 shows the comparison between the predicted results and the experimental results. The results show that the model that assesses the carbon conversion factor has RSM = 11.7, while the model with a carbon conversion factor of 1 has RSM = 12.8. That shows that the carbon conversion factor model has a more accurate prediction. In addition, this model also predicts the gasification zone temperature of 630.2°C, which is relatively consistent with the experimental results.

Table 1. *Property of Acacia wood [14]*

Parameter	**Weight percent , %**
Carbon	47.68
Hydrogen	5.17
Oxygen	44.38
Nitrogen	0.37
Other	2.38
Ash	0.3

Table 2. *Comparision between model and experimental result of acacia wood chip at MC=16% and ER=0.3*

Component	**Model present**		**Experimental [14]**
	Non-using the carbon conversion factor	**Using the carbon conversion factor**	
H_2	19.32	20.4	14.77
CO	16.87	15.78	11.81
CH_4	4.526	3.33	1.27
CO_2	15.54	15.67	18.57
N_2	43.75	44.83	53.59
LHV [MJ/nm^3]	5.83	5.38	3.69
Temperature of reduction zone	601°C	630.2°C	630÷670°C

Figure 3 shows the effect of moisture content (MC) on the component of the gas product, LHV_{gas}, and the heat efficiency of acacia wood gasification corresponding to ER=0.25. The tendency of the gas components is shown in Figure 3a. The results show the H_2, CH_4, and CO_2 components increase while CO decreases follow uptrend MC. The possible explanation for this tendency is that an increase in the MC increases the H_2O content in the gasification zone, which leads to an increased shift reaction. Figure 3b shows that when MC increases from 10 to 30%, the heat efficiency decreases from 68.88 to 51.92%, LHV_{gas} reduces from 6.02 to 5.65 MJ/nm^3. This remark is consistent with the report [11].

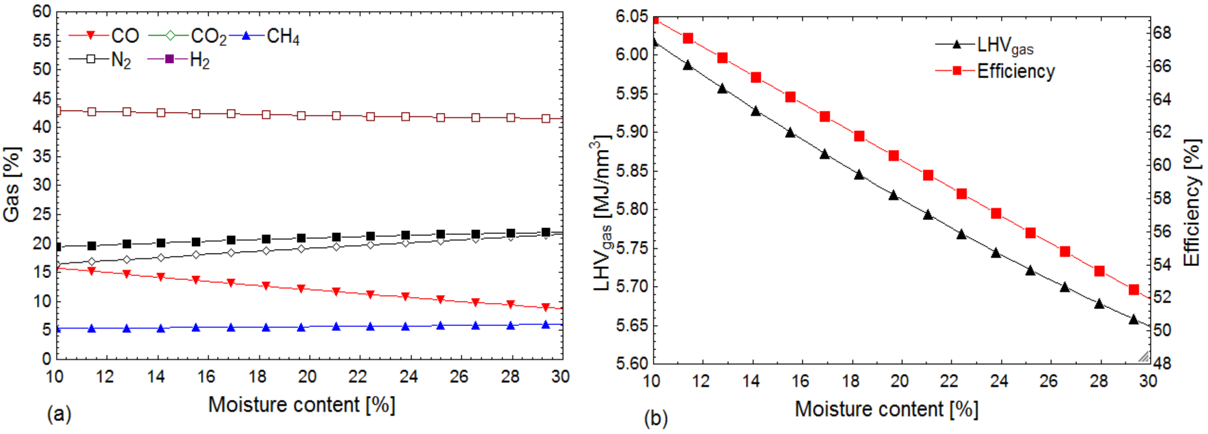


Figure 3. *Effect of MC on gasification: (a) Effect of MC on the component of the gas product; (b) Effect of MC on* LHV_{gas} *and the heat efficiency of the gasifier*

The effect of ER on acacia wood gasification in case MC=20% can be seen in Figure 4. The result shows that the CH_4 and CO_2 components decrease while CO increases with an increase in ER. The H_2 composition increased slightly initially, then decreased with increasing ER (see Figure 4a). It can be explained that by increasing the ER, the gasification temperature increases, thereby increasing the carbon conversion factor and increasing the CO generation reaction. Moreover, the gasification process tends to switch to combustion, so the component gas H_2 and CH_4 decreases. The increase of CO does not compensate for the decrease of CH_4 and H_2, leading to LHV_{gas} tending to decrease when ER is increased. It is in good agreement with the conclusions of previous studies [6] - [7]. Increasing the ER from 0.21 to 0.374, the heat efficiency tends to increase and decrease if the ER continues to increase. It shows that with increasing ER, the number of moles of the product gas increases a lot while LHV_{gas} decreases less, leading to heat efficiency increases. ER increases over 0.374, the gasification process shifts powerfully to combustion, so the number of moles of the product gas increases less while LHVgas decreases more, so heat efficiency tends to decrease. In detail, Figure 4b shows the heat efficiency increased from 57.61 to 63.76% when ER increased from 0.21 to 0.374, then decreased to 63.51% when ER increased to 0.4; LHV_{gas} reduced from 6.29 to 4.51 MJ/nm^3 when ER increased from 0.21 to 0.4.

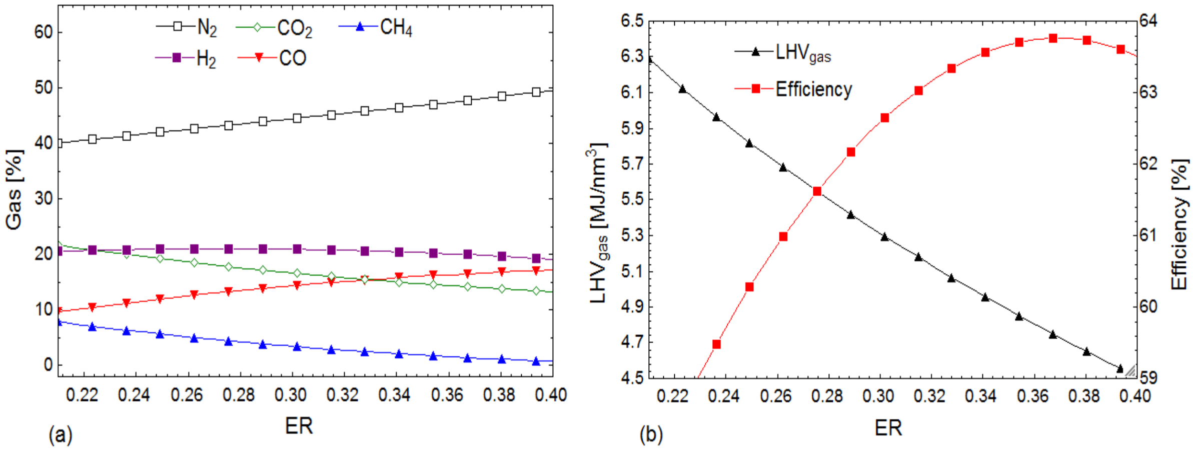


Figure 4. *Effect of ER on gasification: (a) Effect of ER on the component of the gas product; (b) Effect of ER on* LHV_{gas} *and the heat efficiency of the gasifier*

Figure 5 exposes the overall influence of MC and ER on carbon conversion factor (CCF). The influence of MC on CCF is negligible. ER has a significant influence on CCF. It can explain that ER increases, increased oxygen content, accelerated carbon oxidation lead to CCF increases. The carbon conversion factor is from 0.812 to 0.997.

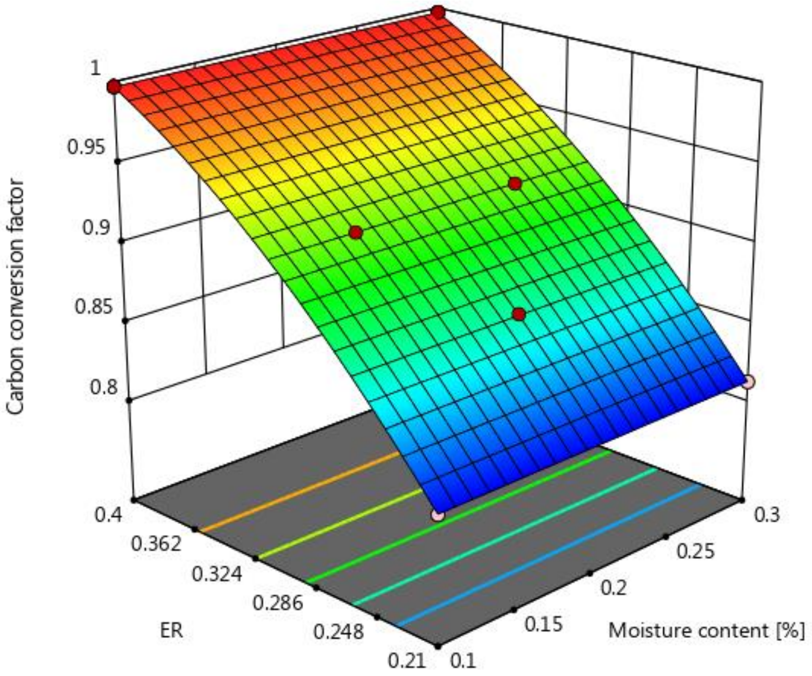


Figure 5. *Effect of MC and ER on carbon conversion factor (CCF)*

Figure 6 shows the variation of LHV_{gas} in the survey range with MC=10÷30% and ER=0.21÷0.4. The results show that LHV_{gas} is maximum when MC approaches 0.1 and ER approaches 0.21. LHV_{gas} has a value from 4.51 MJ/nm^3 to 6.51 MJ/nm^3.

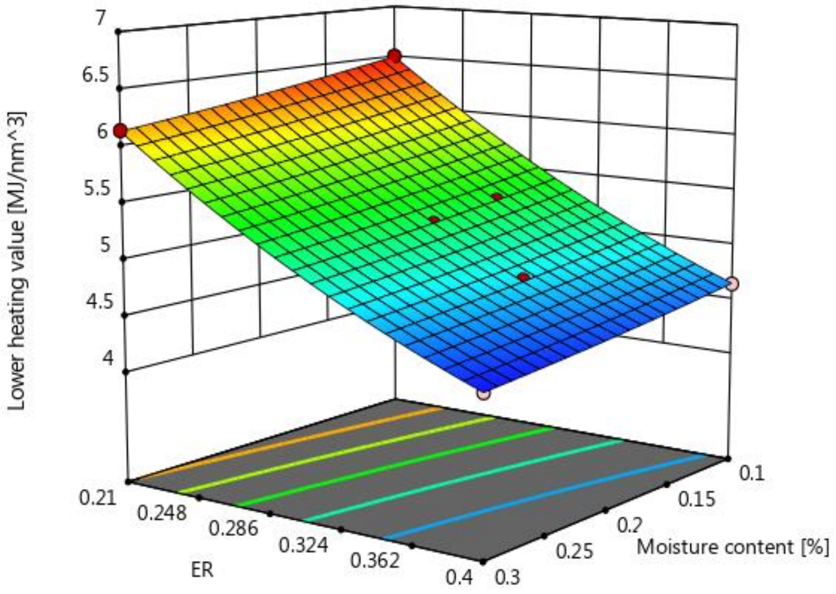
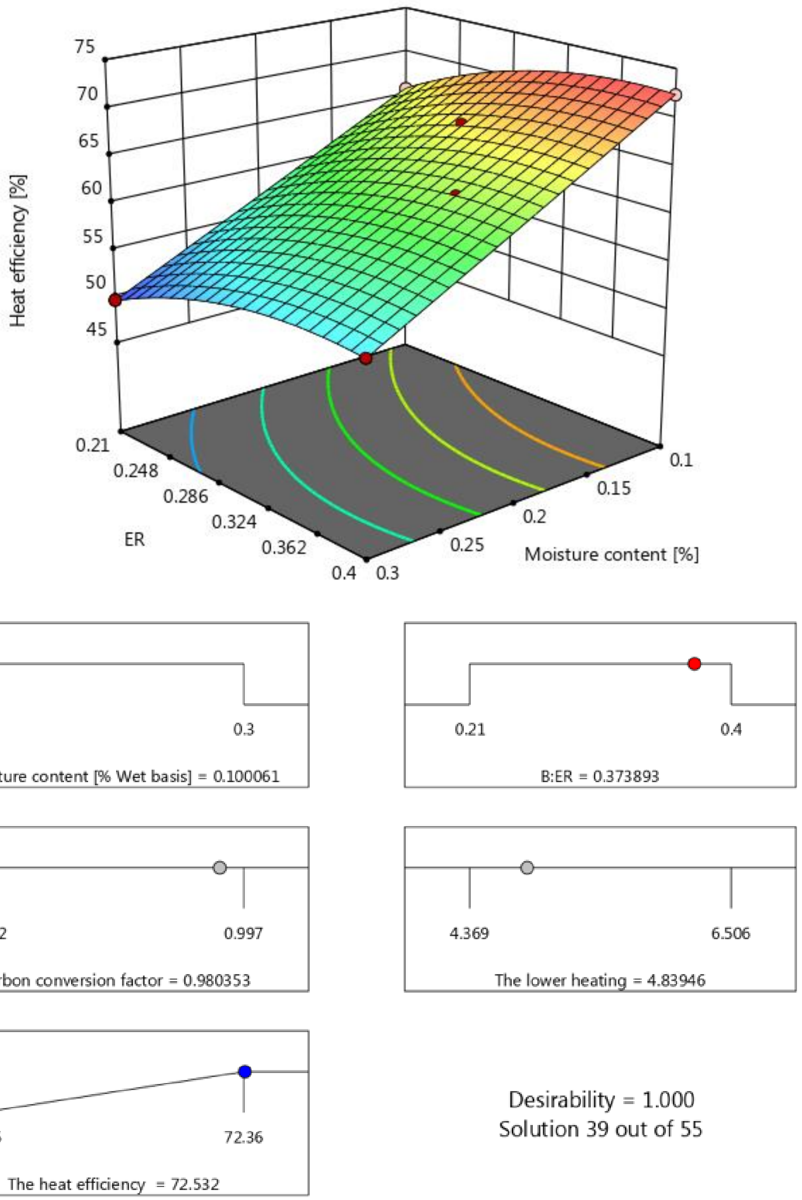


Figure 6. *Effect of MC and ER on the lower heating value (LHV_{gas})*

Figure 7 shows the variation of the heat efficiency of the gasification process. The results show that the heat efficiency is maximal when MC approaches 0.1 and ER approaches 0.374 (results analyzed by Design-Expert software). The heat efficiency has a value from 49.62 to 72.53%. This is entirely consistent with the previous analysis.



This mode- The heat efficiency reaches maximum.

Figure 7. *Effect of MC and ER on the heat efficiency of the gasifier (η)*

4. Conclusions

This study presents a prediction of acacia wood of Vietnam gasification founded the thermodynamic equilibrium model in a downdraft gasifier. The main findings are as follows:

- When MC increased from 10 to 30%, the content of H_2, CH_4, CO_2 increased, the content of CO decreased.

- When ER increased from 0.21 to 0.4, the content of CH_4 and CO_2 decreased, the content of CO increased, the content of H_2 initially increased slightly then tended to decrease.

- The carbon conversion factor increased with increased MC or increased ER. The effect of MC on the carbon conversion factor is negligible.

- LHV_{gas} and heat efficiency decreased with increased MC or increased ER. In the scope of the survey with ER=0.21 ÷ 0.4**,** MC=10 ÷ 30% then LHV_{gas} = 4.51 ÷ 6.51 MJ/nm^3, η=49.62 ÷ 75.53%.

- An equilibrium model can be used to predict gasification for research and teaching on biomass gasification.

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