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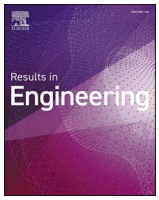

Multi-factor optimization of bio-methanol production through gasification process via statistical methodology coupled with genetic algorithm

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ABSTRACT

This work innovatively explores the bio-methanol production process, conducts comprehensive analyses, develops statistical models, and optimizes operational conditions, contributing valuable insights to the field of sustainable energy production from biomass. Accordingly, bio-methanol production from biomass through gasification route was investigated and simulated using Aspen Plus software. The effects of operational parameters on energy duty of gasification reactor and the methanol production rate in syngas to methanol reactor were investigated. The parameters affecting the process performance including temperature, pressure, and steam/feed ratio were examined using the response surface methodology (RSM) by central composite design (CCD) technique. Analysis of variance (ANOVA) was performed, and two quadratic models were derived. The predicted R^2 values of these models for methanol mass flowrate and energy duty were 0.9394 and 0.9363, respectively. The optimal operational conditions were identified using genetic algorithm (GA). The optimum values of temperature, pressure, and steam/feed ratio in gasification reactor were 900 °C, 4 bar, and 0.675, respectively. This condition leads to methanol mass flowrate and energy duty of 4.254 kg/s and 40736.355 kw, respectively. In addition, sensitivity analysis was performed on syngas to methanol reactor performance.

1. Introduction

In recent years, due to the phenomenon of global warming, air pollution, and energy crisis, efforts such as upgrading fossil fuels [1–3] or replacing them with renewable energy sources [4–6] have been undertaken. Combustion of bio-methanol as a renewable energy results in lower emissions of gases such as nitrogen oxide, carbon dioxide, and sulfur oxide compared to fossil fuels [7]. The reduction of greenhouse gas emissions, the possibility of using it in internal combustion engines with minor modifications [8,9], and the availability of multiple sources as feedstock for its production are among the advantages of using bio-methanol as a green fuel.

Despite the above mentioned advantages, the production and use of bio-methanol as a green fuel are also accompanied by several disadvantages. The need for land to cultivate biomass for bio-methanol production leads to an increase in food prices and ultimately poses a threat to food security, especially for poor countries. Therefore, the production of bio-methanol from the waste biomass such as agricultural residues, food waste, and stabilized sewage sludge can be useful solutions. Further, during the process of producing this bio-fuel, formaldehyde gases and nitrogen oxides are generated, which lead to environmental pollution. The release of these gases is also among the other disadvantages of this green fuel production.

Bio-methanol can be produced through both biological and chemical methods. In the chemical process, due to the use of a catalyst, the efficiency of the process is higher. Furthermore, process control is easier in chemical methods, leading to higher productivity. Due to better process control and higher efficiency in chemical processes compared to biological ones, there is a greater inclination towards industrial-scale production of bio-methanol using chemical methods.

Zheng et al. investigated the gasification process of several woody biomass sources for the production of bio-methanol. They simulated this process using Aspen Plus simulator. Further, they assessed the economic profitability of this process. They reported that biochar is the best biomass with the highest production efficiency [10]. AlNouss et al. performed a techno-economic analysis of bio-methanol production

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through gasification of palm oil waste as biomass. Further, they assessed the impact of CaO addition on CO_2 capturing during the gasification and advancing the process performance. They used Aspen Plus as simulation environment and conducting economic evaluation by this software. Finally, they investigated the effects of parameters on process performance through doing sensitivity analysis [11]. Im-orb et al. investigated the gasification of oil palm residues using a model in Aspen Plus. They reported that the highest gasification performance is achieved when temperature and equivalent ratio are 750 °C and 0.25, respectively [12].

In gasification process, the gasifying agent can be air, oxygen, or steam [4]. AlNouss et al. compared the gasification process with pure oxygen only and steam only as gasifying agents. They concluded that the use of steam as gasifying agent is economically and environmentally preferable to pure oxygen [13]. Liu investigated the gasification of coal, biomass, and coal/biomass with air/steam gasifying agent with Aspen Plus simulator. The results showed that coal gasification is more cost-effective for methanol production in comparison with the other two feedstocks [14]. Of course, it should be noted that in the economic evaluation of a process, various factors such as energy prices, availability of feedstocks, tax laws, and so on, have impact. Therefore, over time and with changing conditions, a process that is currently cost-effective may not be economically viable in the future, and vice versa. Furthermore, a cost-effective project in one region may not be economically viable in another geographical area. In addition, in bio-methanol production, one should not only consider economic issues. Rather, the production of bio-methanol is also important from environmental perspectives.

Yousef et al. used fuzzy logic methodology to develop models to predict yield of bio-methanol production from sugar cane bagasse. The operative parameters were reaction temperature, reaction time, and nitrogen flow. They reported good agreement between model predicted and real data. In addition, they used particle swarm optimization (PSO) technique to find the optimum values of operational parameters [15]. Shamsul et al. investigated the optimization of bio-methanol production from goat manure via statistical approach. The operational parameters included temperature, hydraulic retention time (HRT), and cell concentration [16].

Countries with significant amounts of agricultural and food waste or any other type of non-utilizable biomass waste should pay special attention to the production of bio-methanol and investment in this field.

Mathematical modeling is a critical tool to examine the influencing parameters and can be used to forecast the process performance and optimization [17,18]. But in some cases, developing a precise mathematical model is hard and impossible due to the lack of knowledge in nature of process. Design of experiment (DoE) method is a practical tool for examining the effect of various operational parameters on process performance. The advantage of this method over the conventional method is considering the interaction between operational parameters and performing fewer tests, which leads to time savings and reduced testing costs. Given the popularity and effectiveness of this approach, DoE is used in various studies in different fields of science and technology [19–28].

In this study, the whole biomass gasification process for bio-methanol production was investigated and evaluated. Due to the existence of multiple main sections and different units in the plant, it is not possible to thoroughly examine, study the effect of operational parameters, model, and optimize all the equipment and units in one paper. Therefore, in this study, the focus is on simulation, modeling, and optimization of the gasification and syngas to methanol process. Totally, the gasification process is of great importance in bio-methanol production. So, the effects of operational parameters on energy duty of gasification reactor and the production rate of syngas to methanol process were investigated. Accordingly, in first step, the whole process was simulated using Aspen Plus software. Then, the parameters affecting the performance of process including temperature, pressure, and steam/feed ratio in gasification reactor were examined using the DoE-RSM central composite design (CCD) technique. Analysis of variance (ANOVA) was performed, and statistical models were derived. In the next step, optimal conditions for the process were obtained using the developed models and genetic algorithm (GA) as optimization algorithm. In addition, sensitivity analysis was performed on syngas to methanol reactor performance. The impact of temperature and pressure on methanol mass flowrate and mass fraction in output were investigated.

This study brings innovation to the forefront by delving into the production of bio-methanol from biomass via the gasification route. Through a combination of in-depth parameter analysis, process simulation, statistical modeling, RSM, sensitivity analysis, and optimization techniques, authors offer novel insights into the realm of sustainable energy production from biomass. The models developed in this work have acceptable accuracy. These findings pave the way for enhanced efficiency and environmental sustainability in methanol production, contributing to the broader field of renewable energy solutions.

2. Methods and materials

2.1. Process mechanism

The production process consists of three steps including dehumidification, syngas production, and methanol production from syngas. In bio-methanol production through gasification route, biomass is converted to syngas, mainly including CO,H_2, CO_2, and CH_4, then syngas is converted to methanol in a catalytic process [29]. The reactions of syngas production in gasification and pyrolysis, which reported by Moghadam et al. are as follows [30]:

$$C+1/2O_2 \rightarrow CO \text{ Exothermic} \quad (1)$$

$$C + O_2 \rightarrow CO_2 \text{ Exothermic} \quad (2)$$

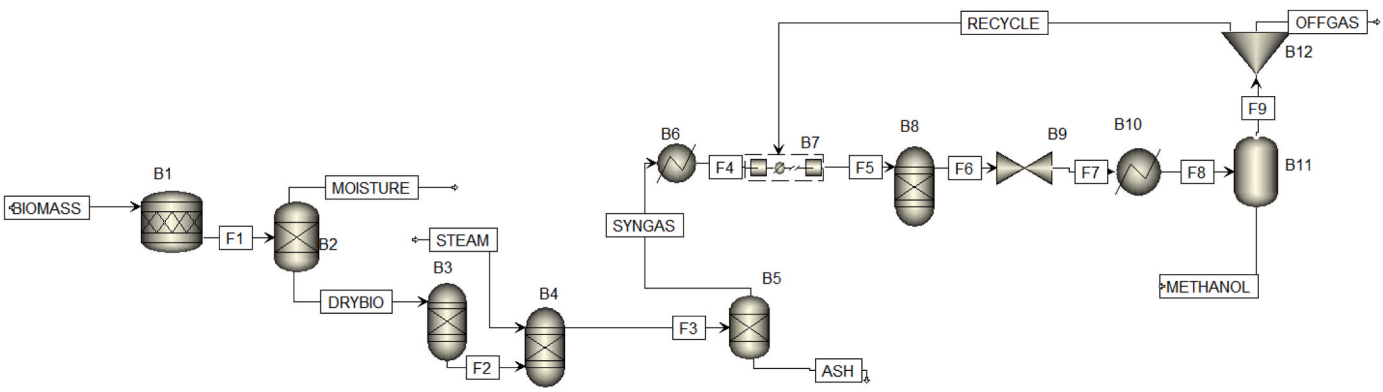

Fig. 1. PFD of biomass to bio-methanol process.

Table 1
Biomass compositions.

Component	Weight Fraction wt% (Dry Basis)
Carbon	51.19
Hydrogen	6.08
Oxygen	41.3
Nitrogen	0.2
Sulfur	0.02
Chlorine	0.05
Ash	1.16

$$C + CO_2 \rightarrow 2CO \text{ Endothermic} \quad (3)$$

$$C + 2H_2 \rightarrow CH_4 \text{ Exothermic} \quad (4)$$

$$C + H_2O \rightarrow CO + H_2 \text{ Endothermic} \quad (5)$$

$$CO + H_2O \rightarrow CO_2 + H_2 \text{ Exothermic} \quad (6)$$

$$CH_4 + H_2O \rightarrow CO + 3H_2 \text{ Endothermic} \quad (7)$$

$$CH_4 + CO_2 \rightarrow 2CO + 2H_2 \text{ Endothermic} \quad (8)$$

$$C + 2H_2O \rightarrow CH_4 + CO_2 \text{ Endothermic} \quad (9)$$

In this work, steam is used as a gasifying agent and the whole process is endothermic.

The reactions that occur in in the process of converting the syngas to methanol (hydrogenation) are as follows [10]:

$$CO + 2H_2O \rightarrow CH_3OH \quad (10)$$

$$CO_2 + 3H_2 \rightarrow CH_3OH + H_2O \quad (11)$$

These reactions are exothermic. Therefore, the operational temperature of reactor should not be high. The pressure and temperature of syngas to methanol conversion were set within 50–150 bar and 200–300 °C, respectively [10].

The output stream from the methanol production reactor consists of methanol, water, and unreacted synthesis gases. In the first step, unreacted syngas are separated from the mixture of water and methanol and is recycled to the inlet of reactor. In the second step, water and methanol need to be separated each other, and pure methanol should be obtained.

2.2. Process description

In Fig. 1, a process flow diagram (PFD) of bio-methanol production process simulated in this work is shown. The specifications of the biomass used in this study are based on the work of Poluzzi et al. [31]. The constituent components of biomass are presented in Table 1. Aspen Plus (version10) software was used to simulate the process. The used fluid package is Peng-Robinson. The pressure, temperature, and flowrate of feedstock are 1 bar, 25 °C, and 10.27 kg/s, respectively. The binary interaction parameters have been shown in Table 2.

In the first step, the biomass should be moistened. For this purpose, the feed is introduced into a stoichiometric reactor called B1. The conversion percentage in this reactor is 0.444 and the reaction is as follows:

$$\text{Biomass(wet)} \rightarrow 0.055508H_2O + \text{Biomass(dry)} \quad (12)$$

In the next stage, the mixture is fed into a separator called B2 in order to separate moisture from dry biomass. In the following, dry biomass is fed into a conversion reactor called B3.In this reactor, biomass is decomposed into its constituent components.

The output products from the B3 reactor are fed into a Gibbs reactor called B4. In this reactor, several products such as CO, CO_2, H_2O, CH_4, HCl, H_2S, and NH_3 are produced.

The output stream from the B4 reactor is fed into a separator called B5.The purpose of installing this separator is to remove ash from the synthesis gases. In the following, the synthesis gases are introduced into a cooler (B6).Then, along with the return flow from the methanol purification section, it enters into a multistage compressor (B7).

In the next step, the high-pressure flow is introduced into a high-pressure Gibbs reactor (B8). In this reactor, synthesis gases are converted into methanol. The output product from the B8 reactor is then fed into a cooler (B10) after passing through a pressure relief valve. And finally, it enters into separator B11. In this separator, methanol is separated from synthesis gases. Totally, 25% of the unreacted synthesis gases are purged, and the rest is recycled to the multi-stage compressor.

The mass flowrate of different components in final product and the return stream are presented in Table 3.

2.3. Design of experiment

Different regression models, including linear, two-factor interaction (2FI), and quadratic, were investigated. These models for three input parameters are presented by equation (13)–(15), respectively.

$$Y = [\alpha_A, \alpha_B, \alpha_C].\begin{bmatrix} A \\ B \\ C \end{bmatrix} + \beta \quad (13)$$

Table 3
The mass flowrate of different component (kg/s).

Component	Recycle	Off Gas	Product
H_2O	0.00410624	0.00136879	0.0512877
H_2	0.192506	0.0641695	3.40E-05
CO	2.99082	0.996934	0.001363
CO_2	8.23422	2.74475	0.125292
CH_4	0.786555	0.262185	0.00167839
NH_3	0.000217607	7.25E-05	3.07E-05
H_2S	0.00302987	0.00100996	0.000203862
N_2	0.0339044	0.0113015	3.39E-05
CH_4OH	0.891725	0.297241	3.74199
HCL	0.00810795	0.00270265	0.000233582

Table 2
The binary interaction parameters.

Component i	Component j	K_{Aij}	Component i	Component j	K_{Aij}
H_2O	CO_2	0.12	CO	N_2	0.0307
H_2O	NH_3	−0.2589	CO_2	CH_4	0.0919
H_2O	H_2S	0.04	CO_2	H_2S	0.0974
H_2O	CH_4O	−0.0778	CO_2	N_2	−0.017
H_2	CO	0.0919	CO_2	CH_4O	0.023
H_2	CO_2	−0.1622	CH_4	N_2	0.0311
H_2	CH_4	0.0156	NH_3	N_2	0.2193
H_2	N_2	0.103	H_2S	N_2	0.1767
CO	CH_4	0.03	N_2	O_2	−0.0119
CO	H_2S	0.0544	N_2	CH_4O	−0.2141

Table 4
The operational range of operative parameters.

Operative Parameters	Operational Range	Unit
Temperature	700–900	°C
Pressure	2–4	bar
Steam/Feed Ratio	0.675-1.225	–

Table 5
The design layout of experiments.

std	run	Temperature (°C)	Pressure (bar)	Volume (m3)
16	1	800	3	0.95
10	2	1000	3	0.95
19	3	800	3	0.95
2	4	900	2	0.675
6	5	900	2	1.225
15	6	800	3	0.95
20	7	800	3	0.95
3	8	700	4	0.675
13	9	800	3	0.4
8	10	900	4	1.225
18	11	800	3	0.95
12	12	800	5	0.95
17	13	800	3	0.95
4	14	900	4	0.675
5	15	700	2	1.225
7	16	700	4	1.225
11	17	800	1	0.95
14	18	800	3	1.5
1	19	700	2	0.675
9	20	600	3	0.95

Table 6
Data specifications.

	Temperature	Pressure	Steam/ Feed	Mass Flowrate	Energy Duty
count	20.00	20.00	20.00	20.00	20.00
mean	800.00	3.00	0.95	3.31	36772.70
std	91.77	0.92	0.25	0.65	6881.87
min	600.00	1.00	0.40	1.97	16635.24
25%	775.00	2.75	0.88	3.05	34487.97
50%	800.00	3.00	0.95	3.52	38954.65
75%	825.00	3.25	1.02	3.64	40132.15
max	1000.00	5.00	1.50	4.27	44790.75

$$Y = \begin{bmatrix} \alpha_A, \alpha_B, \alpha_C \\ \alpha_{AB}, \alpha_{AC}, \alpha_{BC} \end{bmatrix} \cdot \begin{bmatrix} A & AB \\ B & AC \\ C & BC \end{bmatrix} + \beta \tag{14}$$

$$Y = \begin{bmatrix} \alpha_A, \alpha_B, \alpha_C \\ \alpha_{AB}, \alpha_{AC}, \alpha_{BC} \\ \alpha_{A^2}, \alpha_{B^2}, \alpha_{C^2} \end{bmatrix} \cdot \begin{bmatrix} A & AB & A^2 \\ B & AC & B^2 \\ C & BC & C^2 \end{bmatrix} + \beta \tag{15}$$

Where β is the intercept and α is the coefficient of parameters.

By comparing the performance of each of these models in fitting the data, optimal models were selected.One of the important indexes for evaluating the reliability of a model is R^2, but it should be noted that as the operational variables increase, the value of R^2 increases while the predictive power of the model does not necessarily increase. To address this issue, another index called "adjusted R^2" is defined. Although R^2 and adjusted R^2 indicate the predictive power of the model, they are calculated based on the data used for fitting the model. Accordingly, another index called "predictive R^2" is introduced, which has a better performance in introducing an optimal model.

The operational parameters and their ranges of variation are presented in Table 4. The operational range of these parameters has been determined based on the work of other researchers [10]. It should be noted that the developed model will only be valid within a range of operational variables mentioned in this table.

Fig. 2. Correlations between parameters.

Table 7
Determination coefficients of different models.

Response	Model	R^2	Adjusted R^2	Predicted R^2
Bio-methanol Mass Flowrate	Linear	0.7083	0.6536	0.4790
	2FI	0.7710	0.6654	0.5447
	Quadratic	0.9927	0.9861	0.9394
Energy Duty	Linear	0.7512	0.7046	0.5272
	2FI	0.7635	0.6544	0.5274
	Quadratic	0.9923	0.9854	0.9363

In Table 5, the design arrangement of the experiments using the CCD method is presented. Based on the fact that there is three operative parameters and considering six repetitions at center point, the number of experiments will be twenty. It should be noted that the reason for repeating the experiments at the center point is to determine the amount of systematic error in the results.

2.4. Data assessment

Table 6 shows the specifications of the obtained data. Fig. 2 illustrates the correlation between operational variables and the response. The closer the correlation coefficient is to one or minus one, the stronger the correlation between the two variables. It is clear that there is no significant correlation between the operational variables. Mass flowrate has the highest correlation with temperature. Furthermore, the correlation between energy consumption and temperature is even stronger than the correlation between mass flowrate and temperature.

3. Result and discussion

3.1. Model assessment

The data collected in this study were modeled using statistical methods. As mentioned before, regression models were used to establish predictive relationships between the factors and the responses. Various models including linear regression, 2FI, and quadratic regression were studied and investigated. Table 7 displays the values of R^2, adjusted R^2, and predicted R^2 of these models for energy duty and bio-methanol flowrate. It is clear that the best fitted model is quadratic one.

For the statistical analysis, widely accepted methods, including ANOVA were employed. This statistical tool provided the ability to assess the significance of the independent variables and their interactions on the response variables. Backward elimination technique was used to remove unimportant factors from the models. This technique is commonly used in regression analysis. In this way, all potential

Table 8
ANOVA table for reduced models.

Response	Source	df	Sum of Squares	Mean Square	F Value	p-value Prob > F
Bio-methanol Flowrate	Model	7	11.29298	1.613284	199.3214	<0.0001
	A-Temperature	1	7.463097	7.463097	922.0664	<0.0001
	B-Pressure	1	0.372841	0.372841	46.06454	<0.0001
	C-Steam/Feed	1	0.231366	0.231366	28.58528	0.0002
	AB	1	0.239948	0.239948	29.64558	0.0001
	AC	1	0.463635	0.463635	57.28221	<0.0001
	A^2	1	2.502775	2.502775	309.2181	<0.0001
	C^2	1	0.173061	0.173061	21.38166	0.0006
Energy Duty	Model	6	8.900E+008	1.483E+008	196.90	<0.0001
	A-Temperature	1	5.756E+008	5.756E+008	764.06	<0.0001
	B-Pressure	1	7.250E+006	7.250E+006	9.62	0.0084
	C-Steam/Feed	1	9.312E+007	9.312E+007	123.60	<0.0001
	AB	1	8.010E+006	8.010E+006	10.63	0.0062
	AC	1	2.837E+006	2.837E+006	3.77	0.0743
	A^2	1	2.032E+008	2.032E+008	269.73	<0.0001

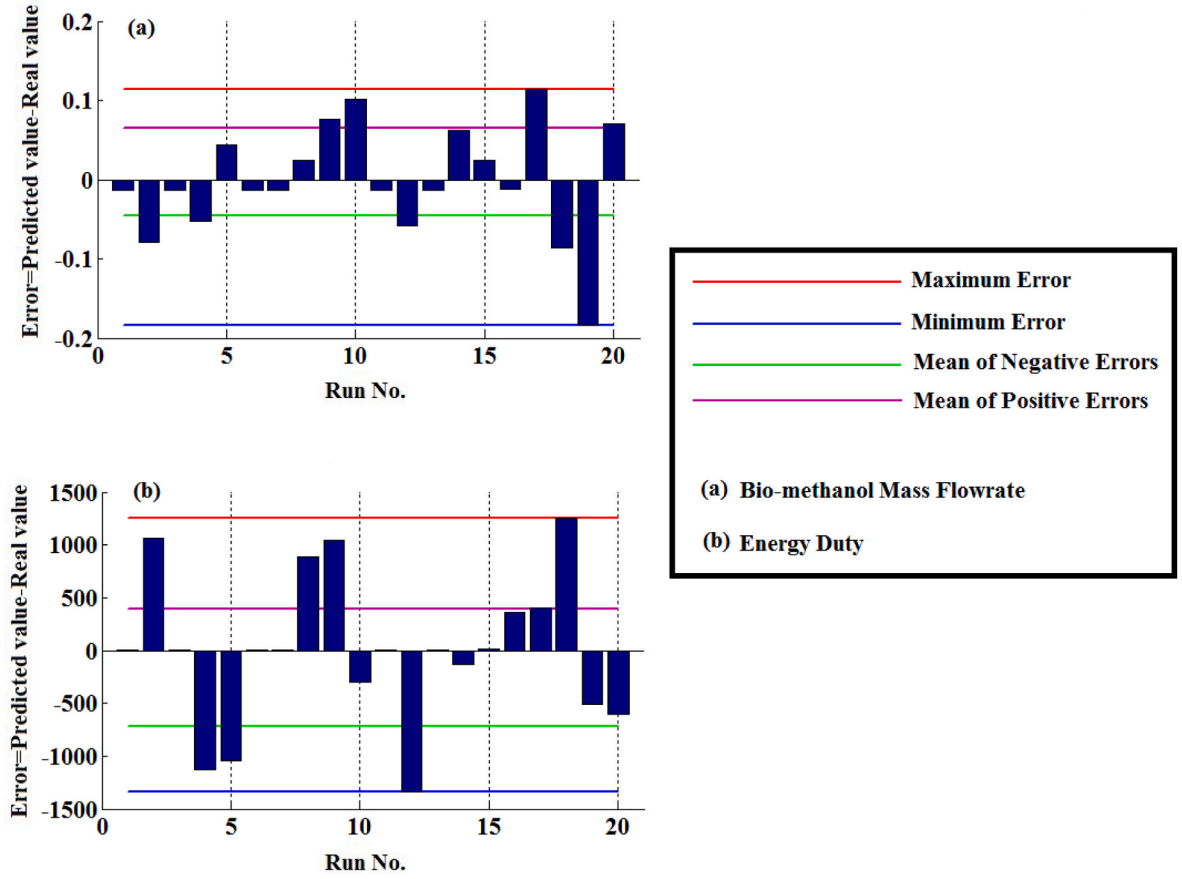

Fig. 3. Estimated errors.

predictive factors and their interactions were included in the model (R^2 values of these models have been shown in Table 7). Then, the significance of each variable and interaction was evaluated systematically and those that did not contribute significantly to explaining the variance in the dependent variables was removed from the model.

Accordingly, BC, and B^2 were removed from model for flowrate and BC, B^2, and C^2 were removed from energy duty model. The p-values of theses interactions were above the predetermined significance level. After removing these ineffective factors, the predicted R^2 of bio-methanol flowrate and energy duty raised to 0.9568 and 0.9572, respectively. It is clear that backward elimination helps simplify the model by retaining only the most relevant factors. The ANOVA table of reduced model has been presented in Table 8.

The reduced statistical models extracted for bio-methanol flowrate and energy duty in coded form are as follows:

$$\text{Bio-methanol Flowrate} = 3.59 + 0.68A - 0.15B - 0.12C + 0.17AB - 0.24AC + 0.038BCE - 0.31A^2 - 0.010B^2 - 0.083C^2 \quad (16)$$

$$\text{Energy Duty} = 38959.34 + 5998.04A - 673.15B + 2412.44C + 1000.59AB - 595.56AC - 2733.30A^2 \quad (17)$$

Based on statistical analysis, the importance level of factors for the bio-methanol flowrate and energy duty are as follows:

Bio-methanol Mass Flowrate: $A > A^2 > AC > B > AB > C > C^2$

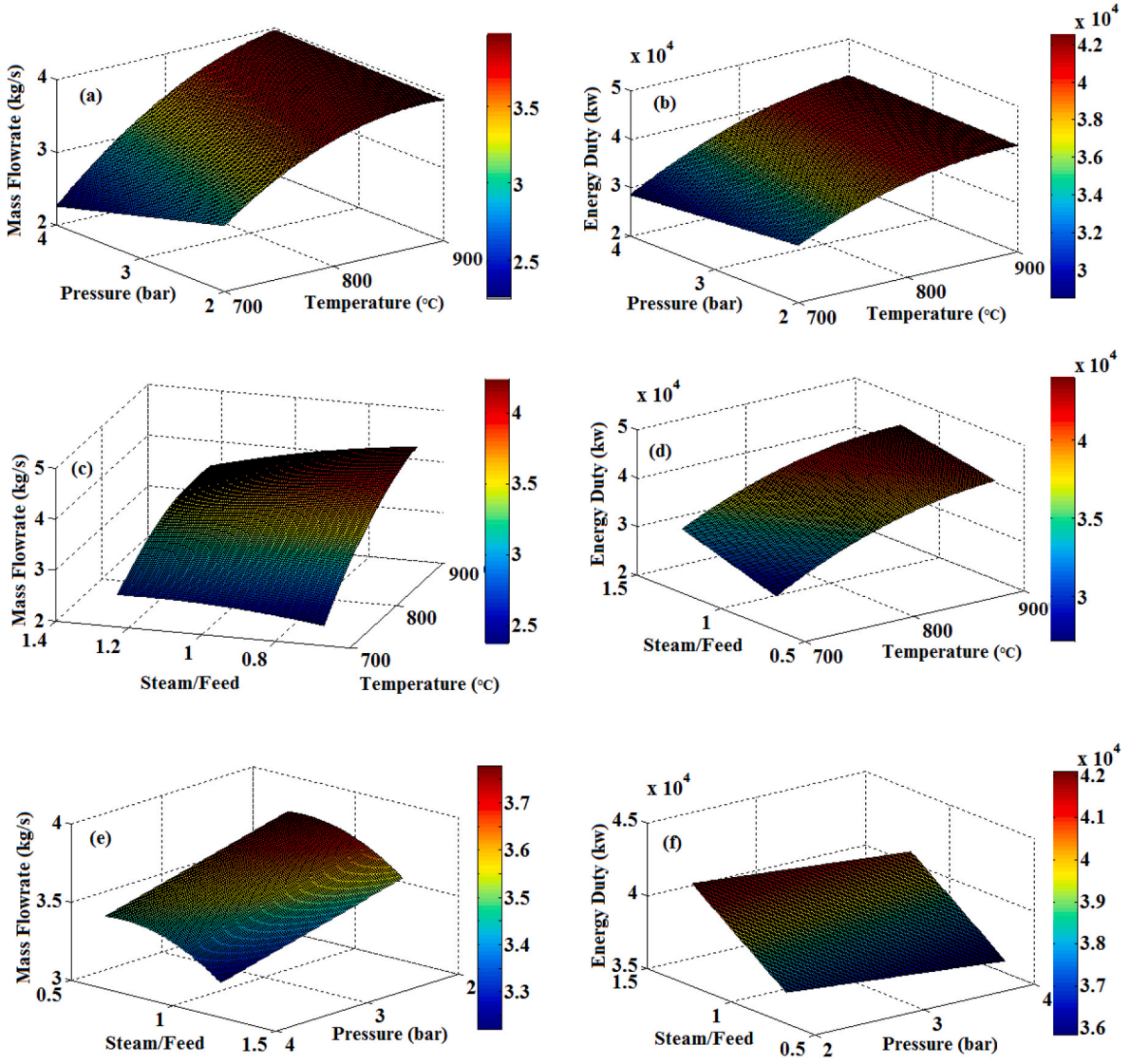

Fig. 4. Predicted mass flowrate and energy duty vs. operative parameters.

Energy Duty: $A > A^2 > C > AB > B > AC$

The "Adeq precision" for bio-methanol mass flowrate and energy duty are 57.538 and 55.187, respectively. This index indicates the capability of the model to extrapolate to new experimental data. If the "Adeq precision" value is greater than 4, it signifies sufficient accuracy of the model in fitting the data and making predictions.

The coefficient of variation (C.V.) was computed, which serves as a measure of the relative variability within the dataset. The calculated C. V. value for mass flowrate and energy duty were 2.75% and 2.36%, respectively. These values signify that the degree of variation in this dataset, relative to the mean, is moderately low. These values of C.V. imply that the data points exhibit relatively consistent values in comparison to the dataset's average. Accordingly, this observation suggests that the dataset is stable, with variations that are not pronounced in relation to the overall mean, supporting the reliability of the findings and conclusions.

In Fig. 3, the estimated error of bio-methanol mass flow rate and energy duty are shown.

3.2. Parametric analysis study

In Fig. 4, the predicted mass flow rate of bio-methanol and energy duty are plotted against the input variables. It should be noted that these charts are plotted based on derived statistical models. In Fig. 4 (a), the values of bio-methanol mass flow rate are plotted against temperature and pressure. Meanwhile, the steam to feed ratio has been kept constant at the average value. As evident, with an increase in temperature, the mass flowrate increases. Furthermore, for higher temperature values, changes in pressure do not have a significant effect on the mass flowrate. However, for lower temperature values, increasing pressure results in a decrease in the mass flowrate. Of course, this decrease is not significant. Such observation also exists for energy duty (Fig. 4b).

Based on Fig. 4 (c), at high temperatures, the decrease in the steam to feed ratio leads to an increase in mass flowrate. However, the decrease in the steam to feed ratio results in a reduction in energy duty (Fig. 4d). In Fig. 4 (d), energy duty is plotted as a function of pressure and steam to feed ratio. Contrary to the previous charts, the relationship between the independent variables and the response is linear, while the extracted statistical relationship is quadratic in nature. The reason for this is that, by fixing the temperature value, the quadratic model for energy duty is transformed into a linear regression model.

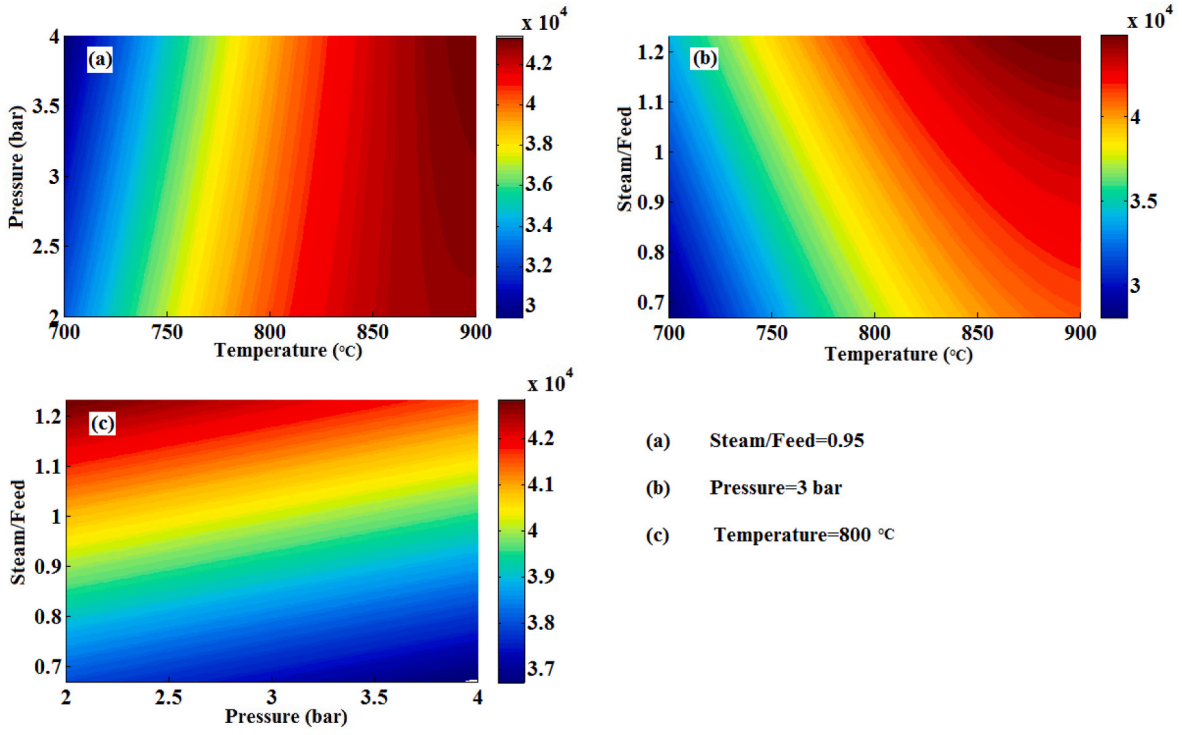

Fig. 5. Optimization function vs. input parameters.

3.3. Optimization

In this research, the optimization process relied on models derived through CCD and GA. Multiple distinct strategies were developed, each assigning varying weights to individual input and output parameters. The optimization process was then carried out based on these strategies. By changing the values of the operational variables, the mass flowrate of bio-methanol and energy duty changes simultaneously. By defining an optimization function and assigning weights to each of the operational variables and responses, optimization can be performed. The defined optimization function is as follows:

$$Optimization\ Function = W.X \tag{18}$$

$$W = \left[w_{Flowrate.}, w_{Energy}, w_{Temp}, w_{Press.}, w_{SF}\right] \tag{19}$$

$$X = \begin{bmatrix} 1-Flowrate \\ Energy\ Duty \\ Temperature \\ Pressure \\ Steam\ to\ Feed\ ratio \end{bmatrix} \tag{20}$$

Where W is the weights assigned to the input and output variables. This optimization function is defined in such a way that the optimal conditions result in the minimum value of the function. A unique weight between zero and unity is assigned to each of the five dependent and independent variables. The closer the assigned weight to a factor is to one, the more important that factor is, and the closer it is to zero, the less important it is.

GA has better performance and higher speed compared to other optimization methods. Therefore, it is used in many optimization applications [32–37]. GA is actually a computational method that uses a combination of biological concepts and mathematics for optimization. The algorithm defines the process environment as a population of individuals with specific characteristics.

In this study, the goal is to find values for the operational parameters that lead to the minimum value of the defined optimization function. In the first step, an initial population is created with random genes. The second step is generating the next generation using genetic operations. The genetic operation includes selecting parents with high fitness, changing chromosomes to improve performance, and creating the next generation using the selected and modified parents. And the third step is evaluating the fitness of each individual, based on which the best individual is selected.

The optimization function is plotted against the operational variables in Fig. 5. In this figure, equal weights have been assigned to all dependent and independent variables. Considering that the independent and dependent parameters differ from each other in terms of values, therefore, equation (18) cannot be used to optimize the process by GA. To face this, all variables involved in the optimization function have been normalized. And the optimization calculations have been performed

Table 9
Optimum conditions.

Strategy No.	Weights	Temperature	Pressure	Steam/Feed	Predicted		Aspen Plus	
					Mass Flowrate	Energy Duty	Mass Flowrate	Energy Duty
1	1-0-0-0-0	900	4	0.675	4.254	40736.355	4.196126	40829.89
2	0-1-0-0-0	700	4	0.675	2.061	25546.338	2.030981	24906.74
3	1-1-1-1-1	700	2	0.676	2.714	28908.361	2.789121	29364.07
4	1-1-0-0-0	899	2	0.676	4.212	40081.770	4.26734	41154.53
5	1-1-1-1-0	700	2	0.680	2.718	28950.333	2.789334	29415.59
6	1-1-0.5-0.5-0	700.6	2	0.675	2.720	28954.554	2.790206	29425.76

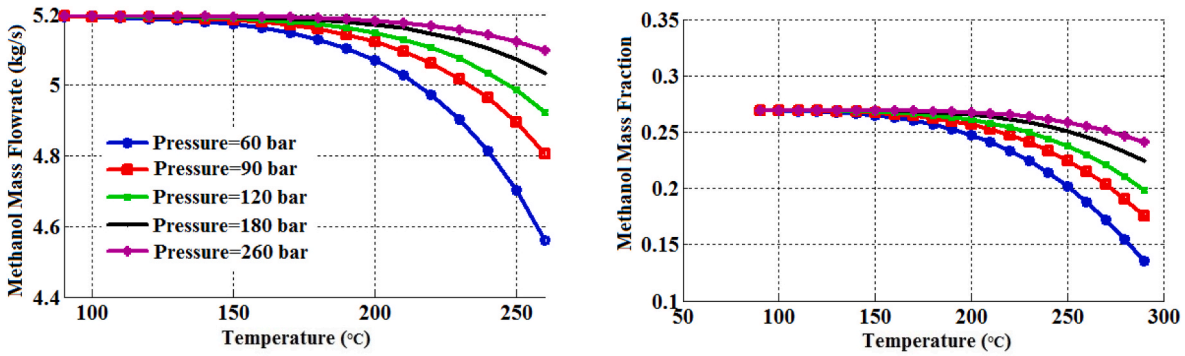

Fig. 6. Methanol to syngas process performance vs. temperature and pressure.

based on the normalized values. The optimum conditions corresponded to different strategies is presented in Table 9. The methanol mass flowrate and energy duty predicted by extracted models as well as Aspen Plus simulator in optimum conditions have been presented in this table. The values of R^2 of this dataset for methanol mass flowrate and energy duty are 0.9942 and 0.9997, respectively.

3.4. Sensitivity analysis

In the process of methanol production from syngas, sensitivity analysis was performed for the mass flowrate and mass fraction of methanol vs. reactor temperature and pressure. The sensitivity analysis of this reactor was performed using the Aspen Plus simulator. Fig. 6 illustrates the variations in methanol mass flowrate and mass fraction as a function of mentioned operative parameters. As it is evident, with an increase in temperature at different pressures, the mass flowrate and mass fraction of methanol at the reactor outlet decrease. This observation is consistent with the exothermic nature of methanol production reactions. Temperature changes between 90 and 150 °C have no significant impact on response variables. Further, at high temperatures, as the pressure of reactor increases, it leads to an increase in the mass flowrate and mass fraction of methanol in reactor outlet.

4. Conclusion

In this study, the bio-methanol production via gasification route was simulated, modeled, and optimized. Based on obtained data from Aspen Plus simulator, statistical models were developed for methanol mass flowrate in outlet of syngas to methanol reactor and energy duty of gasification reactor with R^2 of 0.9923 and 0.9927, respectively. These results imply that the statistical models can fully explain the relations between input and responses. Using these developed models, the effects of operative parameters on the responses were examined. The analysis of variance (ANOVA) revealed that the gasification temperature has the highest impact on energy duty of gasification reactor and the methanol production rate in syngas to methanol reactor. Based on developed statistical models coupled with genetic algorithm (GA), optimization was performed for different strategies. It was figured out that the maximum achievable methanol mass flowrate is 4.254 kg/s.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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