Original Research Article

Simulation and Optimization of Bio-methanol Production from Steam Gasification of Sugarcane Bagasse using Aspen Plus

ABSTRACT

The detrimental environmental impacts of fossil fuels are increasing due to the growing global energy consumption. Thus, energy recovery from waste materials will inevitably become the dominant option in the future with population growth and the reduction in fossil resources. A model for the production of Bio-methanol was developed using Aspen Plus and design of experiment and optimization were carried out using Design Expert software. Factors selected for the design of experiment were the gasification temperature, gasification pressure and steam / biomass ratio with their value ranges of 500 – 800 ^{o}C, 1 - 3 bar and 0.5 - 2.5 respectively. The effects of interaction between the variables and the response were studied using the Box-Behnken design. The developed model was validated using the yield of bio-methanol from experimental data in literature. The model gave bio-methanol yield as 4.54% while the bio-methanol yield from experimental data obtained was 5.93%. The results from Response surface methodology (RSM) gave the quadratic model as best fit for the production of bio-methanol. The coefficient of determination for bio-methanol yield was found to be 0.9435. The optimum gasification conditions were found to be; temperature of 800^{o}C, pressure of bar and steam / feed ratio of 0.5 and these gave rise to the maximum bio-methanol yield of 86.32%. High temperature, low gasification agent (steam/feed ratio) and low pressure favours optimum bio-methanol yield.

Keywords: Response surface methodology, bio-methanol, gasification, biomass, design of experiment, optimization, modelling, simulation

1. INTRODUCTION

Increased demand in fossil fuels for chemicals, fuels, and energy has caused ever-increasing concern for the adverse effects of global warming [1]. Energy production from biomass has been attracting a considerable amount of attention due to concern in energy security and global climate change [2]. Methanol is an important chemical that can be used as a clean burning fuel for replacing the liquid fossil fuel without changing the existing infrastructures. It can also be used as intermediate for the synthesis of numerous chemicals.

Generally, methanol is produced from syngas derived fossil fuels, i.e., partial oxidation of methane, steam reforming of natural gas, or gasification of coal [3], which causes high CO_2 emission during the process. Therefore, the bio-methanol production from syngas through biomass gasification has attracted crescent interest, especially, in agricultural countries [4]. However, the use of biomass for gasification requires large amount of biomass because it has low energy density, which sequentially results in high transportation costs [5].
Biomass is a biological material derived from living, or recently living organisms. It is basically carbon and a mixture of oxygen, nitrogen, hydrogen and also small quantities of other atoms such as alkali, alkaline earth and heavy metals. In addition to being renewable, biomass is considered carbon-neutral [6]. The CO_2 produced during the consumption of

biofuels can be absorbed by biomass through photosynthesis during its growth. This implies that there is no extra carbon released into the atmosphere. If the biomass is supplied sustainably, the carbon neutral cycle resolves the environmental challenges of CO_2 emissions derived from fossil fuel and their dangerous effects on the global climate [7].

Biomass can be converted to biofuels through various pathways. Gasification is considered one of the more promising due to high conversion and energy efficiency [8]. This process consists of partial combustion of biomass to produce a low calorific value gas, synthesis gas or syngas, which is a combination of CO, H_2, CH_4 and CO_2 along with tar (condensable organic compounds) and other contaminants (NH_3, H_2S, etc.) [9]. The syngas can be used for power generation by combustion in power plants, upgraded to high carbon compounds (biodiesel and gasoline) through Fischer–Tropsch and methanol synthesis [10]. The several methods in conventional and new processes for producing of bio-methanol are reported as pyrolysis, gasification, fermentation, electrolysis and photo-electrochemical processes [11].

Gasification is the degradation of carbonaceous organic materials at high temperatures after undergoing thermo-chemical transformation using partial oxygen. Gasification is a clean and efficient process compared to combustion [12]. Gasification is a partial thermochemical process, is considered as the most efficient and cost-effective process to convert lignocellulosic biomass to synthesis gas (syngas), which can be directly used as a fuel or as an intermediate for synthesizing various biochemicals and biofuels. In the gasification process, the biomass reacts with a gasifying agent (oxygen, air, steam, or CO_2) to produce syngas (mainly H_2 and CO) and others (CO_2, CH_4 and high molecular weight compounds known as tar) [12]. Operating conditions such as gasifying temperature and pressure, feed material temperature, equivalent ratio (ER) (a ratio of actual air used in the gasification to the stoichiometric air for complete combustion), and steam-to biomass ratio influence the gasifier performance, which impacts the produced gas composition and biomass conversion efficiency [12].

The main purpose of gasification is to provide a reaction of the carbon in the organic substances with the gasification agents to obtain a gas product with a high heating value (HHV) [6]. Biomass selection is of great importance to achieve successful results in gasification. The basic stages of gasification are drying, pyrolysis, reduction, and oxidation. Gasifying agents include air, steam, oxygen, and carbon dioxide. However, air is typically chosen due to its low cost, resulting in reduced lower heating value syngas. The primary components of syngas produced from biomass gasification are hydrogen and carbon monoxide, but methane, carbon dioxide, water vapour, and nitrogen with different contaminants like ammonia, tars, and hydrogen sulphide are also present [13].

Aspen Plus is used extensively in industry and academia for steady-state and dynamic simulation, process design, performance modelling, and optimization [14]. Aspen Plus provides a comprehensive and integrated solution. It is capable of handling solid, liquid, and vapor phases at any point in the process flow [15]. When modelling a complex process, small aspects of the process can be modelled separately before being combined into the overall process. Moreover, this software is incorporated with a massive internal property data bank. It also comes with various built-in unit operation blocks that simulate certain operation of a process [16].
Response surface methodology (RSM) has been found to be a useful tool to study the interactions of two or more factors [17]. RSM is a collection of mathematical and statistical techniques that are useful for modelling and problems analysis in which a response of interest is influenced by several factors [18]. It is suitable for dealing with multivariant experimental design strategies, statistical modeling and optimization process. Several previous researchers have proved that RSM was a powerful statistical tool in process

optimization [19]. The primary goal of optimization design is to minimize unfavorable or undesired outputs or maximize the desired outputs [18]. Sometimes, simple linear and interaction models are not enough to provide a brilliant picture of the process [20].

The depleting reserves and environmental issues have pushed the world to search for eco-friendly, sustainable, renewable energy sources and with such focus an alternative energy source is bio-fuel. Bio-methanol has a significant role in the current scenario of energy crisis and environmental degradation due to its potentiality and availability. But they are too expensive to seriously compete with fossil fuels because of the high production costs of the high heat energy consumption during the process.

Thus, the needs to reduce these negative impacts by finding the best formula of optimization from various effects that affect bio-methanol production under intense investigation by using the statistical application approach of response surface methodology and Aspen Plus in order to generate the best formulation which produces the highest yield of bio-methanol. Thus, this research seek to develop a model that can predict methanol yield from sugarcane bagasse using Aspen plus [21] and optimize the process conditions using Design Expert software [22].

2. MATERIAL AND METHODS

2.1 Model development

2.1.1 Assumptions

- Biomass feed rate is 75kg/h
- The gasification process was operated under a steady state and the reactions reached chemical equilibrium.
- The product gases from biomass gasification consist of CO, CO_2, H_2, CH_4, H_20, N_2 and NH_3
- The ash is inert and does not participate in chemical reactions [23]
- Only NH_3 is formed and no nitrogen oxide is considered [24, 25, 23]
- Tar and other heavy hydrocarbons are not considered as a Gibbs reactor model has been assumed for the gasification reaction. Tar and heavy hydrocarbons are products of non-equilibrium reactions and thus are not considered in the model [24, 26].

Steam served as a gasification agent in the simulation of a methanol; gasification plant. Some of the operating parameters are gasification temperature, gasification pressure and steam / Biomass ratio. The proximate analysis and ultimate analysis of sugarcane bagasse used are shown in Table 1.

Table 1: Proximate and ultimate analysis of sugarcane bagasse used

Proximate Analysis (wt %)		Ultimate Analysis (wt %)	
Fixed carbon (FC)	4.69*	Carbon	43.53
Volatile matter (VM)	93.50*	Hydrogen	6.12
Moisture content (MC)	7.67	Oxygen	47.33**
Ash	1.81*	Nitrogen	1.21
		Ash	1.81*

Source: [27]

** Calculated on dry basis*

*** Not supplied in the original reference but calculated in this study as 100% -% C -% H -% N -% ash*

The PENG-ROB (peng-robinson) property method was set for this simulation. It is recommended for gas processing, refinery and petrochemical applications which include gas plants, ethylene plants, etc. This property method is suitable for high temperature and pressure regions. PENG-ROB property method is generally used for nonpolar or mildly polar mixtures.

The steam class was set as MIXED, CISOLID and NC (MIXCINC). MIXCINC is used when conventional and nonconventional solids are present, with no particle size distribution. The NC properties: Enthalpy and Density model was selected as HCOALGEN and DCOALIGT, respectively, for dry-feed and ash which are non-conventional components. HCOALGEN is the general coal/SW model for computing enthalpy in the Aspen Physical Property System which includes a number of different correlations for: heat of combustion, heat of formation and heat capacity. The density model, DCOALIGT, gives the true (skeletal or solid-phase) density of coal/SW on a dry basis using ultimate and sulfur analyses.

In the simulation, DRYFEED and ash are defined as a non-conventional component and the DCOALGEN and HCOALGEN models were used to determine the density and enthalpy of the dryfeed. Firstly, the DRYFEED was converted to its conventional elements (H, C, O, N) and ash in a RYIELD reactor, called DECOMP, by specifying the yield distribution according to its ultimate and proximate analyses. Steam was used as the gasifying agent. The gasification reactions were simulated using an RGIBBS reactor, called EQUIL in which the Gibbs free energy minimization approach was applied to estimate the product gas composition. A brief explanation of the unit operation blocks used in the simulation is summarized in Table 2.

The gasification model accuracy was verified by comparing the results of the model with those of reported experiment.

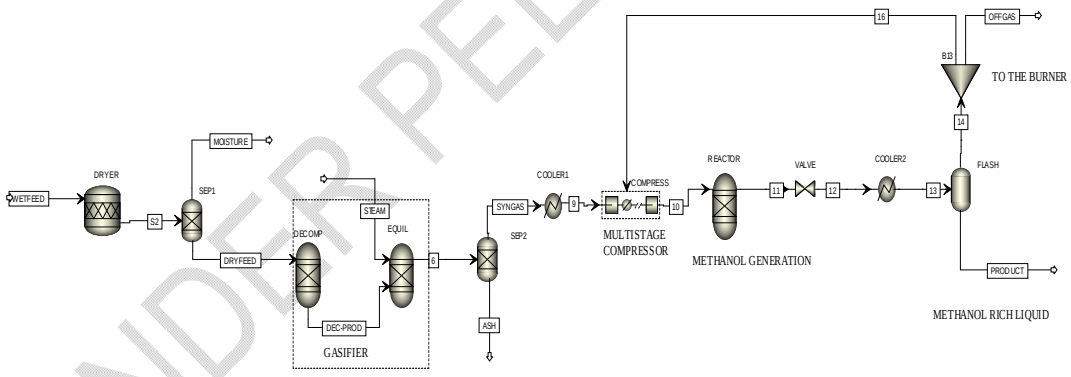

Fig 1: Aspen model flowsheet of the bio-methanol production process

Table 2: Unit operation blocks used to simulate the process

Block name	Block ID	Description
DRYER	RSTOICH	Stoichiometry reactor: Reactor with known conversion rate—used to extract moisture from biomass. Operation at 100^{o}C.
SEP1	SEP	Separator: separation of moisture from the wet feed
DECOMP	RYIELD	Pyrolysis reactor: decomposition of biomass to its constituent components. Operations at 500-800^{o}C
EQUIL	RGIBBS	Gasifier: production of raw syngas through the

		gasification process. Operations at 500-800^{o}C
SEP2	SEP	Separator: separation of ash from the syngas
COOLER1	HEATER	Heat exchanger: decreases the temperature of the syngas gas leaving the separator to 120^{o}C
COMPRESS	MCOMPR	Multistage compressor: increases syngas pressure to 100 bar and decreases temperature to 250^{o}C
REACTOR	RGIBBS	Methanol synthesis reactor: produces raw methanol
VALVE	VALVE	Valve: depressurizes product gas leaving the methanol reactor
COOLER2	HEATER	Heat exchanger: decreases the temperature of the product gas leaving the methanol reactor to 50^{o}C
FLASH	FLASH2	Used to separate part of CO_2 and impurities syngas from methanol and H_2O
B13	FSPLIT	Divides the offgas and H_2O (this is recycled back to the compressor)

2.2 Statistical Analysis

The optimum condition for methanol gasification was determined by Box-Behnken under RSM for the simulations. The independent variables used for the optimization were the gasification temperature, gasification pressure and steam/ biomass ratio. Their respective levels are 500 - 800^{o}C, 1 - 3 bar and 0.5 - 2.5 respectively. The effects of interaction between the variables and the responses were studied using the Box-Behnken design. The coded factor levels are presented in Table 3.

The process conditions values suggested by the design of experiments were used to run the methanol gasification simulations to find their corresponding responses. The various methanol yields were recorded. Numerical optimization of the process variables using RSM in Design Expert software [22] was carried out to maximize bio-methanol yield.

Table 3: Actual levels at coded factor levels of independent variables used in the RSM

Symbol	Independent variable	Actual levels at coded factor levels		
		-1	0	1
A	Temperature (^{o}C)	500	650	800
B	Pressure (bar)	1	2	3
C	Steam/Biomass Ratio	0.5	1.5	2.5

3. RESULTS AND DISCUSSION

3.1 Validation of Results

To validate our process model, the simulation results were compared to experimental data by [27]. The model gave bio-methanol yield to be 4.54% while the experimental was 5.93%. The comparison of our data with the experimental data reported by [27] showed that it agrees.

3.2 Simulated Results

The process variables values suggested by the design of experiments were used to run the bio-methanol gasification simulations to find their corresponding responses. The various bio-methanol yields were recorded as shown in Table 4 and inputted in the software and analyzed. The selection of model and model terms were estimated using Analysis of Variance (ANOVA) in Table 5. Quadratic model for adequacy using ANOVA was used. The fit summary is shown in Table 6

Table 4: The bio-methanol yield obtained from simulation

		Factor 1	Factor 2	Factor 3	Response 1
Std	Run	A:Gasification Temperature	B:Gasification Pressure	C:Steam/ Feed Ratio	Bio-methanol Yield
		Celsius	Bar	Ratio	%
16	1	650	2	1.5	13.93
15	2	650	2	1.5	13.93
7	3	500	2	2.5	1.75
9	4	650	1	0.5	68.13
2	5	800	1	1.5	16.79
3	6	500	3	1.5	1.69
11	7	650	1	2.5	5.82
13	8	650	2	1.5	13.93
14	9	650	2	1.5	13.93
4	10	800	3	1.5	16.6
1	11	500	1	1.5	4.54
10	12	650	3	0.5	44.22
5	13	500	2	0.5	4.38
17	14	650	2	1.5	13.93
12	15	650	3	2.5	5.28
8	16	800	2	2.5	5.9
6	17	800	2	0.5	78.88

Table 4 shows that experimental run 17 gave the maximum bio-methanol yield of 78.88% at gasification temperature of 800^{o}C, gasification pressure of 2 Bars and steam/ feed ratio of 0.5.

The empirical relationship between the bio-methanol yield response and the independent variables is given in Equation 1. A, B and C are coded terms used for gasification temperature, gasification pressure and steam/ feed ratio.

Methanol yield = -166.85243 + 0.606472A – 23.30167B – 2.2125C + 0.004433AB
– 0.11725AC + 5.84250BC – 0.00027A^2 + 2.055B^2 + 14.8775C^2 Equation 1

The factors of the model are represented by constant terms A, B, and C (linear terms), AB, AC, and BC (interactive terms), and A^2, B^2, and C^2 (quadratic terms). A, B, and C are coded terms used for gasification temperature, gasification pressure and steam/ feed ratio respectively. These equations are for identifying the relative impact of the factors by comparing the factor coefficients. In Equation 1, coefficient of interactive factor BC (5.8425) is much higher than the coefficient of A (0.606472), which shows that for the region studied, the BC factor influences bio-methanol yield more than A interaction. The coefficients of one factor represent the effect of that particular factor; the coefficients of more than one factor represent the effect of the interaction between those factors; and the coefficients of the

squared factor represent the quadratic effect of that particular factor. The positive sign in front of the terms indicates a synergistic effect, while the negative sign indicates the antagonistic effect of the factor [28].

Table 5: ANOVA for estimating the significance of the model for bio-methanol yield

Source	Sum of Squares	Df	Mean Square	F-value	p-value	
Model	7857.28	9	873.03	12.98	0.0014	Significant
A-Gasification Temperature	1399.47	1	1399.47	20.80	0.0026	
B-Gasification Pressure	94.46	1	94.46	1.40	0.2747	
C-Steam / Feed Ratio	3909.93	1	3909.93	58.12	0.0001	
AB	1.77	1	1.77	0.0263	0.8758	
AC	1237.28	1	1237.28	18.39	0.0036	
BC	136.54	1	136.54	2.03	0.1973	
A^2	155.65	1	155.65	2.31	0.1720	
B^2	17.78	1	17.78	0.2643	0.6230	
C^2	931.96	1	931.96	13.85	0.0074	
Residual	470.88	7	67.27			
Cor Total	8328.16	16				

Analysis of variance was applied for estimating the significance of the model at the 5% significance level [29]. ANOVA was used to estimate the statistical parameters (R^2, Adjusted R^2, and predicted R^2) of the steam gasification process. Table 5 shows the ANOVA table for the bio-methanol yield response surface quadratic model for the steam gasification process. A more significant matching coefficient is shown by a greater F-value and a smaller p-value (prob. > F) [30]. If the p-value (significance probability value) is less than 0.05, a model term is considered significant. The model is significant, as shown by the F-value of 12.98 bio-methanol yield-responses and p-value of 0.14% (that is, a 0.14% chance that an F-value this large could occur due to noise). Additionally, the bio-methanol-model terms (A, C, AC and C^2) in Table 5 have p-values that are less than 0.05, indicating that they are significant model terms.

Table 6: Statistical parameters for bio-methanol yield

Response	Bio-methanol Yield
R^2	0.9435
Adjusted R^2	0.8708
Predicted R^2	0.0954
Adequate Precision	13.2060

The coefficient of determination for bio-methanol yield (R^2 = 0.9435) as shown in Table 6 is high and close to 1; the adjusted R^2 values (0.8708) for the bio-methanol response is not in reasonable agreement with the predicted R^2 values (0.0954), since the difference is more than 0.2 which may be due to too many terms in the model. The adequate precision that measures the signal-to-noise ratio is greater than for the response (13.206). All of these validations showed that the simulated data for bio-methanol production from the steam gasification process matched the model's projected value accurately.

3.3 Interaction Effects of Input Parameters

Three- dimensional plot (3D plot) and contour plot were generated by Design- Expert software Ver 13. The 3D and the contour plots are used to estimate the effects of the combination of independent variables (gasification temperature, gasification pressure and steam/ feed ratio) on the response (bio-methanol yield).

Figures 2, 3 and 4 are 3D depicts the independent variable's combined effect on bio-methanol yield

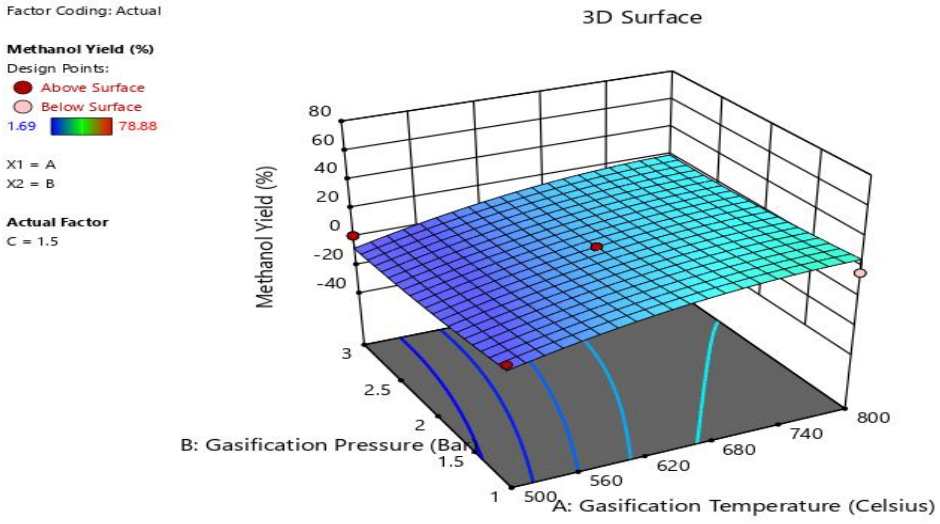

Fig. 2. 3D Plot showing the effect of gasification temperature and gasification pressure on bio-methanol yield response

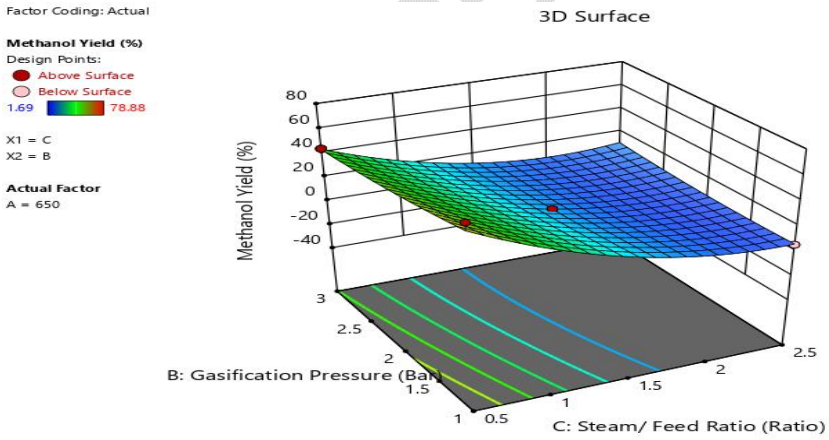

Fig. 3. 3D Plot showing the effect of steam/ feed ratio and gasification pressure on bio-methanol yield response

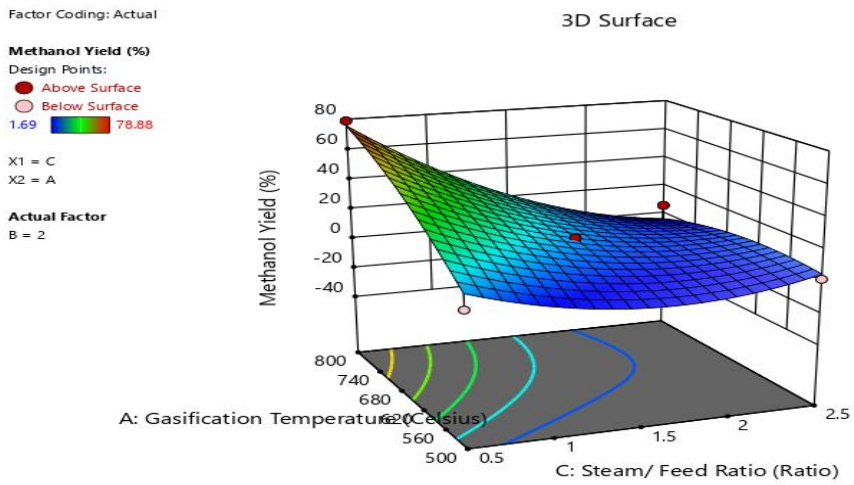

Fig. 4. 3D Plot showing the effect of gasification temperature and steam/ feed ratio on bio-methanol yield response

The effect of gasification temperature and Steam/ feed ratio on bio-methanol yield at the center level of the gasification pressure is shown in Figure 4. The bio-methanol increased as the gasification temperature (A) and steam/ feed ratio (C) decreased at a constant gasification pressure of 2 Bars. The combined effect of gasification temperature (A) and gasification pressure (B) on bio-methanol yield at the center level of the steam/ feed ratio of 1.5 is shown in Figure 2. The results show that increasing A and decreasing B increased methanol yield. Figures 2 and 3 show an increase in bio-methanol yield as the temperature rises. This may be due to Le Chatelier's principle (an increase in temperature favors the forward reaction of an endothermic reaction). Figure 3 indicates the effect of the steam/ feed ratio (C) and gasification pressure (B) on methanol yield at the center level of the gasification temperature of 650^{o}C. It can be seen from Figure 3 that bio-methanol increased as B decreased and C decreased at a constant gasification temperature of 650^{o}C.

3.4 Numerical Optimization

The operating parameters of bio-methanol production process were optimized numerically with the Design Expert [22] to obtain optimal parameters and responses. All the operating parameters are in range. The optimization aimed at increasing bio-methanol yield and 45 solutions of optimization were presented.

Table 7: Optimum response and operating parameters values

Number	Gasification Temperature (^{o}C)	Gasification Pressure (bar)	Steam/ Feed Ratio (Ratio)	Bio-methanol Yield (%)	Desirability
1	800.000	1.000	0.500	86.320	1.000

The highest desirability for the optimization was 1.000 for bio-methanol yield. The desirability function approach transforms the properties of each predicted response to a dimensionless desirability value (d), the dimensionless desirability values range between d = 0 to 1. When d = 0, it suggests that the predicted value is unacceptable and when d = 1, it means that the value is exactly the target value. The value of d increases as the desirability of the corresponding response increases [31].

The optimum operating parameters that increased methanol yield from 78.88% to 86.32% are 800^{o}C, 1bar and 0.5 steam/ feed ratio. The optimization was able to maximize methanol yield.

4. CONCLUSION

Sugarcane bagasse is a potential feedstock for producing transportation fuels because it is readily available. Simulation of bio-methanol production from biomass gasification was carried out, using Aspen Plus Ver. 11 software and Design Expert Ver. 13 software for the optimization of the process. At optimum gasification process variables parameters, bio-methanol yield was maximized of the Response Surface Methodology (RSM). The effects of the three operating parameter; gasification temperature, gasification pressure and steam/feed ratio and their interactions on bio-methanol yield was studied. The optimum methanol yield was 86.32%. The optimum parameters are 800^{o}C (temperature), 1 Bar (pressure) and 0.5 (steam/ feed ratio). It was found high temperature, low gasification agent (steam/feed ratio) and low-pressure favours bio-methanol yield.

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