SIMULATION AND OPTIMISATION FOR PRODUCTION OF BIOGAS FROM PALM OIL MILL EFFLUENT (POME) USING ASPEN PLUS

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ABSTRACT

POME undergoes anaerobic digestion to produce biogas, and when it is purified, the biomass can be used as a fuel. This work aims to create a model to simulate the production of biogas and identify the key parameters of the water scrubber using Aspen Plus. The production of biogas was successfully simulated with a relative difference of less than 5%. The key parameters of scrubber in order of percentage contribution to the purity of biogas is as follows, the temperature of water (38.34%), column pressure (35.29%), water flow rate (23.75%) and lastly, number of stages (2.62%). By employing the optimum values, biogas with 99.3% methane purity was obtained.

Keywords: *Palm oil mill effluent, biogas upgradation, water scrubbing, Aspen Plus, optimisation*

INTRODUCTION

Palm oil mill effluent (POME) is one of the by-products alongside with empty fruit bunch, palm kernel shells, and so on, from the production of crude palm oil in palm oil mill [1]. It is a significant biomass source from palm oil producer such Malaysia, which if it is utilized correctly, it can have a big impact for the overall carbon emission reduction strategy [2]. Palm oil processing in the oil extraction usually gives rise to highly polluting wastewater, known as POME that often ends up discarded in disposal ponds. Fresh POME is a thick brownish colloidal mixture of water, oil, and fine suspended solids which possess a very high Biochemical Oxygen Demand (BOD) and chemical oxygen demand (COD) [3]. The characteristics of POME is tabulated in Table 1.

The approximate production of POME in 2017 is 48,288,080 m^3 and 43,345,568 $m^{3,}$ respectively in West Malaysia and East Malaysia [4]. Biogas is a type of biofuel that is naturally produced from the decomposition of organic biomass waste via anaerobic digestion.

Table 1 Characteristics of POME [3]

Parameter	POME (Average)	Range
pH	4.2	3.4-5.2
Oil and grease	4,000	-
Biochemical oxygen demand (BOD)	25,000	10,250-43,750
Chemical oxygen demand (COD)	51,000	15,000-100,000
Total solids	40,000	11,500-79,000
Suspended solids	18,000	5,000-54,000
Total volatile solids	34,000	9,000-72,000
Ammonical nitrogen (NH_3-N)	35	4-80
Total nitrogen (T.N.)	750	180-1400

As one of the bioenergy type, biogas is continuously available on the production side [5]. Biogas consists primarily of methane (50-75%), carbon dioxide (25-45%), hydrogen sulphide (<1%), and other trace elements. These impurities, especially carbon dioxide and hydrogen sulphide need to be removed from the biogas because they reduce the heating value of the biogas significantly [6]. Currently, one of the most commonly used biogas purification methods is water scrubbing due to its low operating cost and high methane recovery. The purified biogas is used as a fuel for combustion engines to generate electricity while waste heat from engine oil and water-cooling systems and the exhaust could be recovered using a combined heat and power system [7].

The study of the process parameters that affect the water scrubber is very important for the scrubber's design. Understanding of how the process parameters affect the water scrubber and the key parameters in water scrubber are necessary for operators to control and to ensure the scrubber system works efficiently to upgrade the biogas [8]. Previous studies have not mentioned and explained the individual parameters' effectson the water scrubber efficiency. A good simulation model that is able to represent and predict the actual process is essential for researchers for future work, such as further optimising the process before applying changes to the real process.

The main objective of the research project is to model and simulate the production of biogas from POME using Aspen Plus; to simulate and integrate the purification process with the developed biogas production model; to identify and optimise the key parameters of the overall process with emphasis on purification. The main scope of studies for this research project is the modelling and simulation of biogas production plant using POME as feedstock. The types of purification method and their respective advantages and disadvantages are studied to select the best purification method for the upgradation of biogas produced.

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Lastly, the improvement that could be made to the purification process selected is also studied.

METHODOLOGY

The methodology for this research work is divided into two parts; part A: Simulation of biogas production; part B: Optimisation of the purification process of biogas.

Stoichiometry Reaction Method

In part A, the calculation of volume and composition of biogas produced can be calculated by using stoichiometric reactions, following the concept of the component based on the description of the process as implemented in the models of the other process steps [9]. The stoichiometry reaction of these major components namely dextrose, N-Hexadecanoic acid, and protein soluble is as shown in equation 1, 2, and 3 respectively. By using the stoichiometry reaction method, the volume and composition of biogas by the conversion factor for different components can be calculated.

For dextrose $C_6H_{12}O_6$, the reaction is represented by,

$$C_6H_{12}O_6 \rightarrow 3CH_6 + 3CO_2 \quad (1)$$

For N-Hexadecanoic acid $C_{16}H_{32}O_2$, the reaction is represented by,

$$C_{16}H_{32}O_2 + 7H_2O \rightarrow 11.5CH_6 + 4.5CO_2 \quad (2)$$

For protein soluble $C_{13}H_{25}O_7N_3S$, the reaction is represented by,

$$C_{13}H_{25}O_7N_3S + 6H_2O \rightarrow 6.5CH_6 + 6.5CO_2 + 3NH_3 + H_2S \quad (3)$$

Process Simulation of Aspen Plus

Aspen Plus is a software used widely in the world by engineers for the simulation of chemical processes. It is a very all-around tool that is used by engineers, especially for petrochemical processes prediction. Aspen Plus has a source which contains a large list of chemical compounds with their respective thermodynamic properties and the compound's data [10]. NRTL is selected as the property method for this process as it is able to correlate and calculate the mole fractions and activity coefficients of different compounds [11]. POME can be modelled into four components, namely dextrose, N-hexadecanoic acid, protein soluble, and water. The anaerobic digester is modelled using a RSTOIC in Aspen Plus that only requires the user to define the reaction stoichiometry and fractional conversion. The purification of biogas is done using a water scrubber, modelled as RADFRAC without reboiler and condenser [12]. According to the process flow diagram, all the required blocks are constructed, and their operational data as referred to literature is inserted.

Key Parameter Identification and Process Parameter Optimisation

Taguchi Method

In part B, for the identification of key parameters and the optimisation of the parameters, the Taguchi method and ANOVA are employed. Compared to others, the Taguchi method enables parameters can be simultaneously optimised from fewer simulation trials. Two simple tools are being applied, namely signal-to-noise ratio (S/N) and analysis of variance (ANOVA) to determine the optimal conditions and effects of each parameters [13]. Several levels of values have to be assigned to the parameters first. The primary factors most likely to affect the process were determined first, and the range of values for those factors was obtained from the literature. By applying Taguchi Method, the optimum level and value of the parameter out can be deduced [14].

Signal-to-Noise (S/N) Ratio

The signals indicate the effects of process parameters on the process output variable, while noises are calculated by the influence on the deviations from the average responses [14]. The S/N ratio can be categorized into 2 types; "larger is better" and "smaller is better". Since the process output variable, the mass flow rate of carbon dioxide in the bio-methane stream is desired to be minimized, the S/N ratio for each simulation runs was calculated as given by:

For "Smaller is better",

$$\frac{S}{N} = -10 \log_{10} \frac{1}{n} \sum_{i=1}^{n} Y_i^2 \quad (4)$$

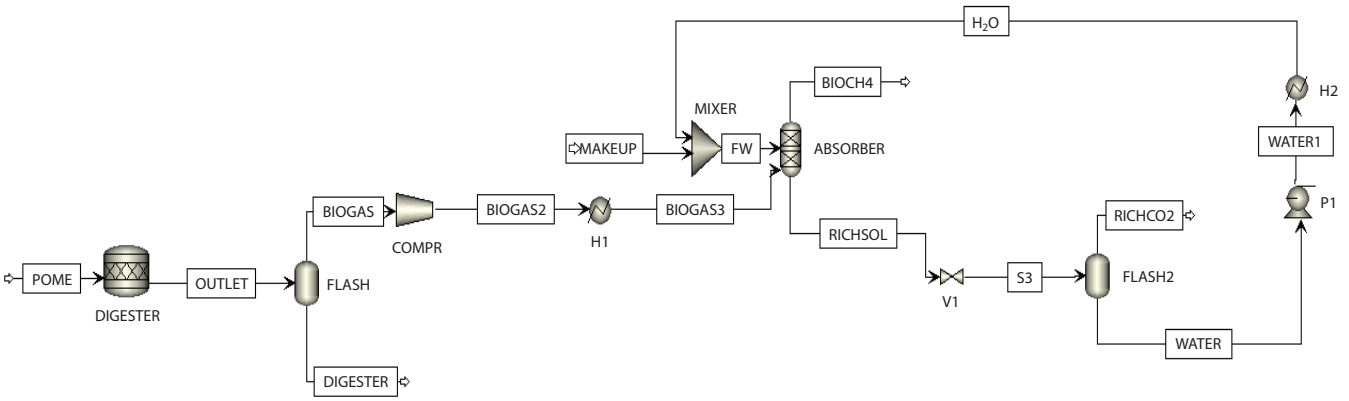


Figure 1 Process flow sheet diagram of production of high purity biogas

Where n is the number of repetitions or observations, and Y_i is the observed output variable. The parameter levels that correspond to the highest *S/N* ratio were selected and considered the optimum condition for the process output variable. The process output variable was observed and recorded.

Orthogonal Array

The Taguchi method uses a special set of arrays called orthogonal arrays. The arrays are able to stipulate the way of conducting minimal number of experiments while being able to obtain the full information on the parameter's effects on the process output variable [15]. For instance, when there are four different independent variables with each variable having 3 sets of values (3^4), categorized into three levels; "Level 1", "Level 2," and "Level 3", a L_9 orthogonal array is selected since L_9 orthogonal array is able to study the effect of 4 variables with 3 sets of values. A L_9 orthogonal array is illustrated below in Figure 2.

Run	A	B	C	D
1	1	1	1	1
2	1	2	2	2
3	1	3	3	3
4	2	1	2	3
5	2	2	3	1
6	2	3	1	2
7	3	1	3	2
8	3	2	1	3
9	3	3	2	1

Figure 2 Standard L_9 (3^4) Orthogonal Array (15)

ANOVA

ANOVA is a computational technique to quantitatively estimate the relative contribution of each process parameter to the process output variable [16]. After deciding the optimum level and optimum value for each factor, ANOVA is performed to analyze the effects of the process parameters. The basic concept of ANOVA is that the total variation is equal to the sum of squares of standard deviation caused by each parameter, as given by [17]:

$$\sigma_T^2 = \sigma_A^2 + \sigma_B^2 + \sigma_C^2 + \sigma_D^2 \quad (5)$$

For each experiment or simulation run, the *S/N* ratio is calculated from the process output variable. For instance, if there is 9 simulation runs, there are 9 *S/N* ratio corresponding to each run. The overall means or the average *S/N* ratio of all the 9 runs is calculated as:

$$S/N_{avg} = \frac{1}{n}\sum_{i=1}^{n} S/N_i \quad (6)$$

Then the level average of *S/N* for each parameter at the level 1 is calculated. For instance, the level 1 value of parameter A appeared thrice in runs 1, 2 and 3, respectively. Therefore, the average *S/N* ratio of the 3 runs of parameter A at level 1 is calculated. The same procedure is repeated for each parameter at each level. By deducting S/N_{avg} from level average *S/N*, the variation caused by the parameter at that level is calculated. Total variation caused by the *i* parameter is calculated by adding all the variation caused by the *i* parameter at every level. For instance, for parameter *i*, the sum of squares due to variation around overall mean is formulated as:

$$SS_i = n_{i1}(SN_{avg,i1} - S/N_{avg})_2 + n_{i2}(S/N_{avg,i2} - S/N_{avg})^2 + ni_3(S/N_{avg,i3} - S/N_{avg})^2 \quad (7)$$

Where n_{i1} is the number of experiment or simulation conducted at level 1 of parameter *i* and $S/N_{avg,i1}$ is the level average response for parameter *i* at level 1. Similarly, this is repeated for all the parameters, and the total sum of squares due to variation around overall mean can be calculated by adding all the parameter's sum of squares. Lastly, the percentage contribution of every parameter to process output variable can be calculated using the formula as given by:

$$Percenage\ contribution\ of\ parameter\ i = \frac{SS_{parameter\ i}}{SS_{total}} \quad (8)$$

Validation of data

The simulation result of part A is validated by comparing the result with the literature result. The result is considered valid when the relative difference is lower than 5%. After part A is completed, the simulation continues up to part B, and the result of part B is validated by ensuringb that the final biogas produced has methane purity over 96%. This is because the minimum requirement for the utilization of biogas as fuel in Malaysia is 96% methane purity [18].

RESULT AND DISCUSSION

Modelling for Production of Biogas

Table 2 shows the result of the simulation for the production of biogas from POME using the stoichiometric reaction method. The amount of biogas and purity of CH_4 are obtained from the simulation and compared with the literature result [11]. The relative difference is calculated.

Table 2 Comparison between simulation and literature

Parameter	Simulation	Literature	Relative Diff (%)
Feed Stream (cum/day)	585	585	-
Biogas Production Rate (m^3/d)	611	603	1.30
CH_4 (% mass)	57.5	55.8	3.04
Temperature	35	35	-

From the result obtained, it can be seen that the results from simulation do not differ much from the literature's result. The relative difference of biogas production rate and mass purity of CH_4 between simulation and literature results is only 1.3% and 3.04%, respectively. The relative difference is well within the maximum tolerance of error of 5%. The stoichiometric reaction method, by using the Buswell equation and its extended equation, is able to calculate the biogas production rate and the composition of the biogas [9]. Based on these results, the model is able to readily simulate the production of biogas from POME and is able to represent the real industrial production of biogas from POME.

Sensitivity Analysis

Four process parameters namely water flow rate, column pressure, water temperature and number of scrubber stages, were identified based on [6] and [11]. These parameters were varied in the ranges which are suitable with part B of this study. The parameter's effect on the scrubber removal efficiency of CH_4 from CO_2 is studied in this section.

Water Flow Rate

Sensitivity analysis was carried out to study the effect of water flow rate on the absorption of CO_2 by water. Other parameters such as temperature, pressure, number of stages, and so on are fixed while the water flow rate is varied from 1 to 6000 kg/hr. The graph of sensitivity analysis obtained from Aspen Plus is as illustrated in Figure 3.

As observed from the graph, the mass flow rate of both CH_4 and CO_2 leaving at the top of the water scrubber reduces as the flow rate of water increases. However, it can be seen that the reduction of the flow rate of CO_2 is more significant than the reduction of the flow rate of CH_4. At the given range of water flow rate from 0 to 6000 kg/hr, the reduction of CH_4 flow rate is only 0.277%, while the reduction of CO_2 flow rate is 91.11%. This is because the solubility of CO_2 in water is much higher than that of CH_4 in water. The purity of CH_4 in biogas increases significantly as the freshwater flow rate increases, as illustrated in Figure 3.

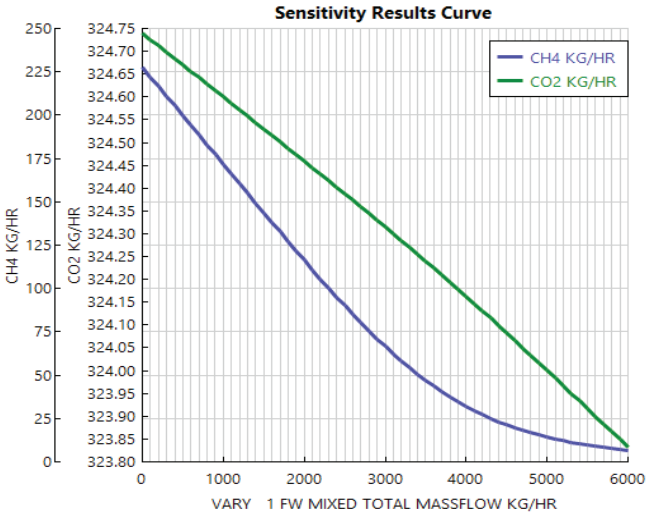
The reason for the reduction of the mass flow rate of CO_2 was attributed to the increased quantity of water flowing through the biogas that has a high composition of CO_2 in it. A high concentration of water molecule and higher intensity of contact between the water molecule and CO_2 molecule increases the reaction of carbon dioxide between water to form carbonic acid as shown in equation 9 [19]. This observation supports the finding from recent study [19] that the increase in liquid molecules can enhance the solvent's bulk absorption capacity.

$$CO_2(g) + H_2O(l) \longrightarrow H_2CO_3(aq) \quad (9)$$

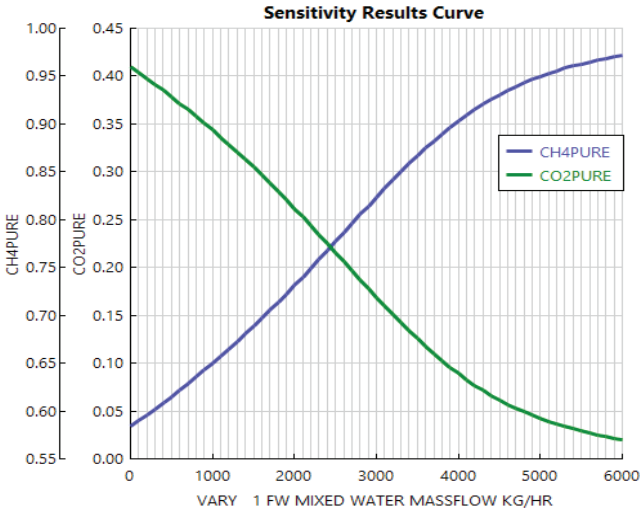
Column Pressure

The effect of column pressure was studied in this section. Other parameters such as temperature, water flow rate, number of stages, and so on are fixed while the column pressure is varied from 1 to 10 bar. The effect of the column pressure on the mass flow and mass purity of CH_4 and CO_2 is as seen below in Figure 4.

As the column pressure increases, the absorption efficiency of water increases, increasing the purity of methane in biogas produced by removing CO_2 from the biogas. The changes in the mass flow of CO_2 are relatively much higher than the mass flow of CH_4 in the final product stream. This observation is also supported by [20] that the CO_2 absorption increases with increasing column pressure. This is because the carbon dioxide's solubility in water increases as the pressure increases [21].

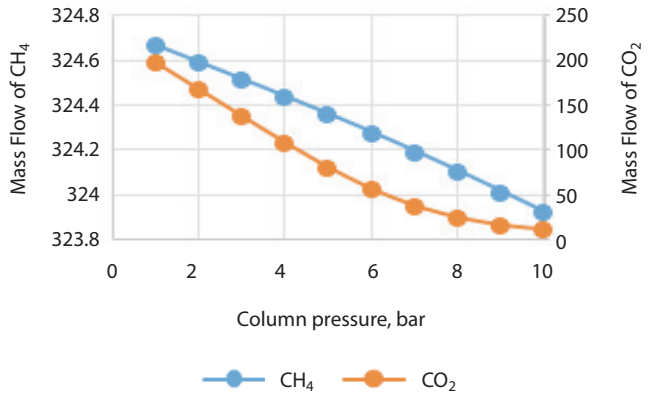


(a) Mass flow rate of CH_4 and CO_2



(b) Mass purity of CH_4 and CO_2

Figure 3 Sensitivity analysis of water flow rate



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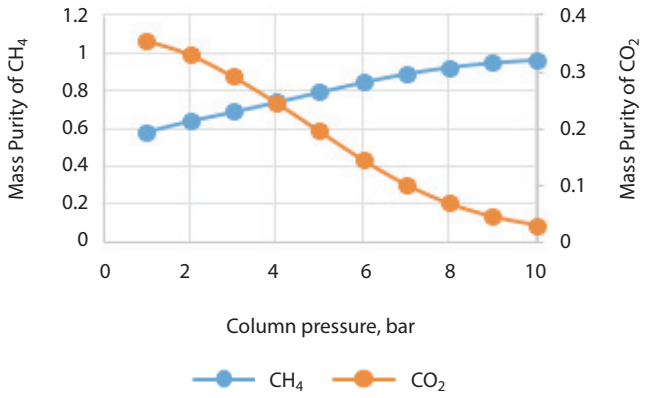


(b) Mass purity of CH_4 and CO_2

Figure 4 Effects of column pressure

Water Temperature

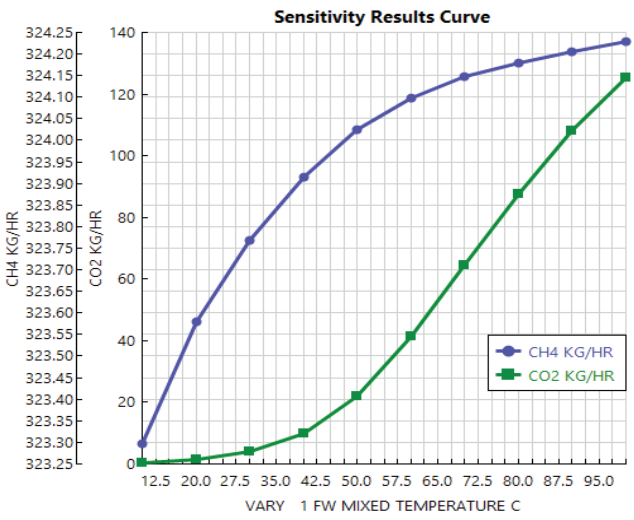
The effect of water temperature is studied in this section, varying temperature from 10°C to 100°C. The result of mass flow rate and mass purity of both CH_4 and CO_2 in the final product stream is obtained and illustrated below in Figure 5.

As seen from the table and graphs, it can be seen that as the temperature of the water increases from 10°C to 100°C, the mass flow rate of CO_2 increases significantly by 99.62% while the mass flow rate of CH_4 increases only by 0.288% in the bio-methane stream. In the bio-methane stream, the mass purity of CH_4 decreases by 34.4% from 99.7% to 65.3%, while the mass purity of CO_2 increases by 25.07% from 0.15% to 25.22%. The absorption efficiency of carbon dioxide by water decreases as the temperature increases because the solubility of carbon dioxide in water decreases. This is because the dissolving reaction of carbon dioxide in water is an exothermic reaction; hence the addition of more heat energy to the system inhibits the forward dissolving reaction of carbon dioxide in water [22]. Therefore, while considering the effect of temperature on CO_2 absorption, water temperature is considered the key parameter because varying water temperature affects the absorption efficiency significantly.

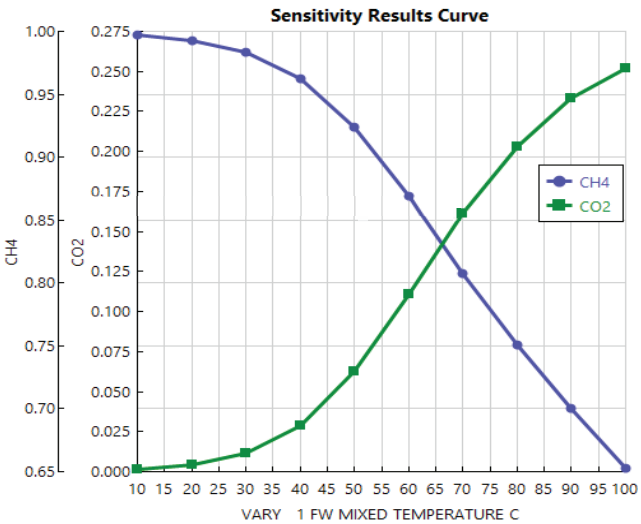
Number of Scrubber Stages

In this section, the effect of the number of stages or the number of trays in the scrubber on the absorption efficiency of carbon dioxide is studied. The number of stages are representing the mass transfer capacities in the scrubber. While leaving all other parameters at constant, the number of stages is varied from 2 to 9.

As seen from the result, the mass flow rate of CH_4 in the bio-methane stream remained almost unchanged increasing only by 0.0079% however, the mass flow rate of CO_2 in the bio-methane stream decreased drastically by 97.13%. The number of stages greatly affects the absorption efficiency of water. For mass purity, the purity

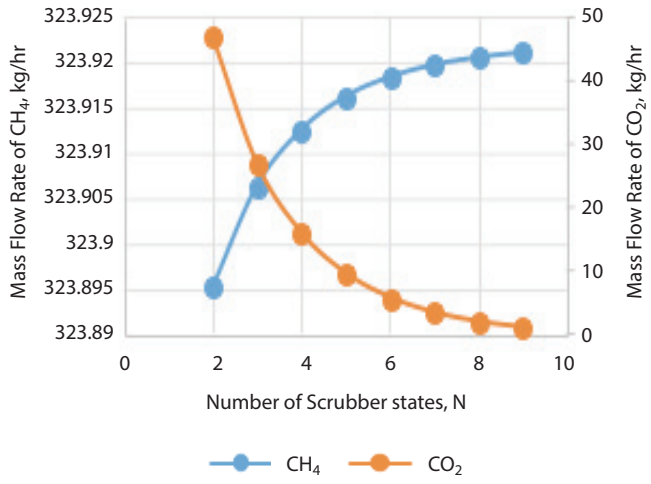


(a) Mass flow rate of CH_4 and CO_2

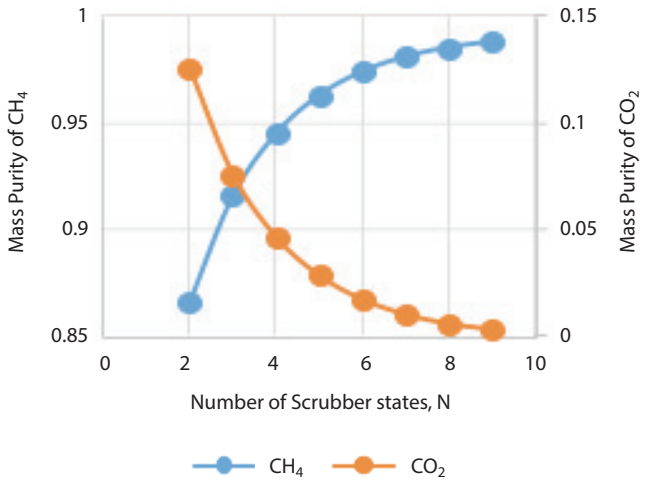


(b) Mass purity of CH_4 and CO_2

Figure 5 Effects of water temperature



(a) Mass flow rate of CH_4 and CO_2



(b) Mass purity of CH_4 and CO_2

Figure 6 Effects of number of scrubber stages

of CO_2 decreases by 12%, while the purity of CH_4 increases by 12% in the bio-methane stream.

Identification of Key Parameters

Since there are 4 different independent variables with each variable having 3 sets of values (3^4), categorized into three levels; "Level 1", "Level 2," and "Level 3", a L_9 orthogonal array is selected since L_9 orthogonal array is able to study the effect of 4 variables with 3 sets of values. The values of the variables were set as shown in Table 3.

Therefore, the independent variables with their respective level values are assigned to the individual column as referred to [15], where four independent variables have been studied and have three levels of values. The simulation of the purification of biogas was conducted for 9 times using 9 different parameter data sets. The process output variable is observed and recorded. Since the process output variable, the mass flow rate of carbon dioxide in the biogas stream is desired to be minimized, the *S/N* ratio for each simulation runs is calculated using equation 4. The process output variable, along with the *S/N* ratio corresponding to each data set are as tabulated below in Table 4.

After computing the *S/N* ratio for each data set, the average *S/N* ratio is calculated for each factor and each level. The average *S/N* ratio corresponding to each factor and level is as tabulated in Table 5 and illustrated in. The main effect is defined as the difference between the largest and smallest *S/N* ratio. The ranking is based on the magnitude of the main effect that indicates which parameter affects the output parameter most.

Therefore, based on the highest S/N ratio, the optimum level, and value for each factor are decided and tabulated in Table 6.

Table 3 Control parameters and levels

Control Parameter	Level 1	Level 2	Level 3
Water Flow Rate, kg/hr (A)	2000	4000	6000
Column Pressure, bar (B)	2	4	8
Water Temperature,°C (C)	20	40	60
Number of stages, N (D)	3	6	9

Table 4 S/N Response table for carbon dioxide flow rate

Run	Independent Variables				Mass Flow rate of CO_2 (kg/hr)	S/N ratio
	A	B	C	D		
1	2000	2	20	3	195.338	-45.816
2	2000	4	40	6	183.033	-45.251
3	2000	8	60	9	164.828	-44.341
4	4000	2	40	9	183.631	-45.279
5	4000	4	60	3	167.818	-44.497
6	4000	8	20	6	11.234	-21.011
7	6000	2	60	6	183.662	-45.280
8	6000	4	20	9	30.391	-29.655
9	6000	8	40	3	36.253	-31.187

Table 5 Average S/N ratio for each factor

Parameter	Level 1	Level 2	Level 3	Main Effect	Rank
A	-45.136	-36.929	-35.374	9.762	3
B	-45.458	-39.801	-32.179	13.279	1
C	-32.160	-40.572	-44.706	12.546	2
D	-40.500	-37.181	-39.758	3.319	4

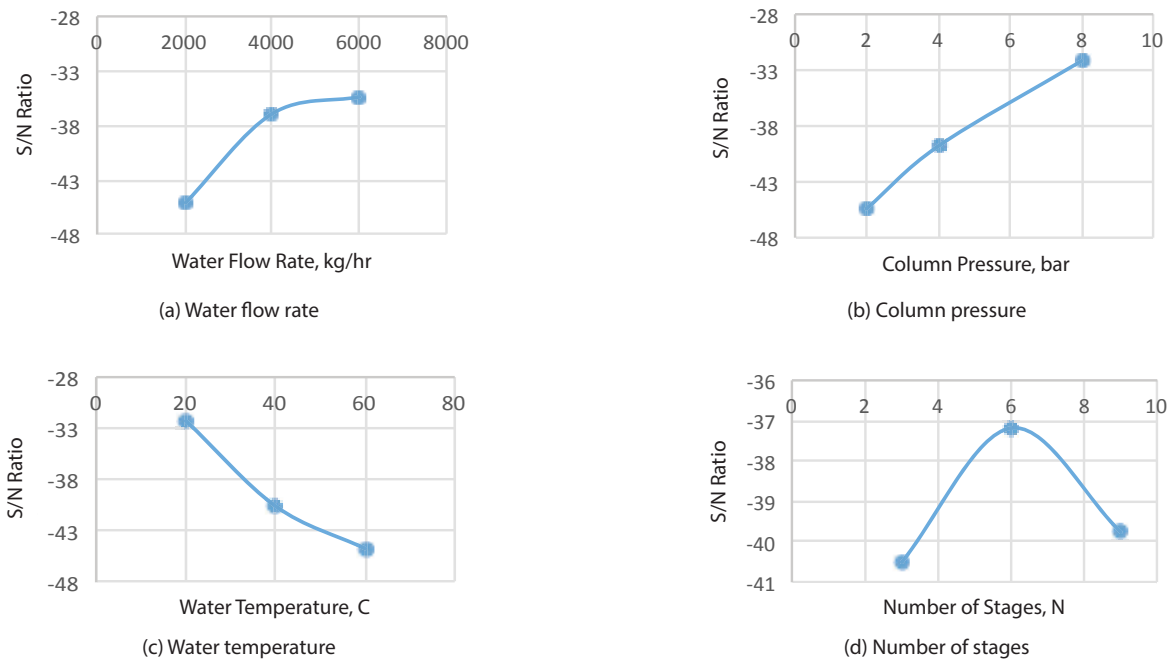


Figure 7 S/N ratio v/s factor level

Table 6 Optimum level and values of each factor

Parameter	Optimum Level	Optimum Value
Water Flow Rate, kg/hr (A)	3	6000
Column Pressure, bar (B)	3	8
Water Temperature,°C (C)	1	20
Number of Stages (D)	2	6

The sum of squares of deviation of each parameter and their contribution percentage is calculated and as tabulated in Table 7.

Therefore, from the result seen above, the highest percentage contribution is from parameter B, "Column Pressure" that contributes 38.34%, followed by parameter C, "Temperature" which contributes 35.29%, and then followed by parameter A, "Water Flow Rate" that contributes 23.75% and lastly parameter D "Number of Stages", that contributes only 2.62%. The effect of the number of stages is considered relatively insignificant while other parameters significantly affect the process output variable.

Table 7 Sum of all squares of deviation of each parameter

Parameter	SS	DOF	Percentage Contribution (%)
Water Flow Rate (A)	165.06	2	23.75
Column Pressure (B)	266.42	2	38.34
Water Temperature (C)	245.24	2	35.29
Number of Stages (D)	18.22	2	2.62
Total	694.93	8	100

Performance Evaluation

By using the optimum level and values of the parameters, a confirmation scrubbing simulation is run again to test the performance of the optimized purification system. The value before scrubbing and after scrubbing is calculated and compared in Table 8.

As seen from Table 8, the purity of methane increased drastically from 57.59% to 99.30% while reducing the purity of carbon dioxide from 40.41% to 0.36% in biogas after using the optimum parameters found using Taguchi Method. The biogas obtained from the simulation complies with the minimum requirements of the utilization of biogas as fuel since 99.30% purity is well over the minimum purity of 96%.

Table 8 Details of biogas before and after scrubbing with optimum process parameters

Gas Content	Before Scrubbing Purity (%)	After Scrubbing Purity (%)	Percentage Improvement (%)
Methane (CH_4)	57.49	99.30	(+) 72.73
Carbon Dioxide (CO_2)	40.41	0.36	(–) 99.11
Water (H_2O)	2.04	0.03	(–) 98.53
Hydrogen Sulphide (H_2S)	0.05	6.73e-07	(–) 99.99
Calorific Value (kJ/m^3)	20581.42	35549.4	(+) 72.73

CONCLUSION AND RECOMMENDATION

It can be concluded that the production of biogas from POME has successfully been modelled in Aspen Plus using the stoichiometry reaction method. The result of the biogas production rate and methane purity is compared to literature data, and the relative difference between this research project's result and literature result [11] is only 1.3% and 3.04% for production rate and methane purity, respectively. Four parameters namely water flow rate, the temperature of water, column pressure, and the number of stages and their effects on the carbon dioxide absorption efficiency, were studied. Based on the results from Taguchi Method and ANOVA, the parameters that affect the purification system significantly followed by their order of percentage contribution are column pressure (38.34%), water temperature (35.29%), water flow rate (23.75%), and the number of scrubber stages (2.62%). The optimum parameters were found out to be 6000 kg/hr for water flow rate, 20 °C for the water temperature, 8 bar for column pressure, and 6 stages for the scrubber. These optimum values for the parameters were applied in the Aspen Plus simulation and the CH_4 purity increased by 72.73%, while for CO_2, H_2O, and H_2S decreased by 99.11%, 98.53%, and 99.99%, respectively compared to raw biogas. The calorific value of the biogas was also calculated and has increased by 72.73% from 20581.42 kJ/m^3 to 72.73% kJ/m^3. Ultimately, by applying these optimum parameters, a 99.3% methane purity of biogas is obtained.

A few recommendations can be suggested to the research project for future works. Firstly, the effects of parameters might change as the amount of biogas scrubbed increases or decreases. The effect of change in the amount of biogas being scrubbed should be studied. Secondly, the electrical energy potential of the biogas produced should be studied as well to determine the optimum values for the parameters for the optimum energy cost ratio. Often, to achieve high purity of biogas requires high energy or high operating cost.

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