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Process Modelling of Microwave-assisted Fast Pyrolysis of Empty Fruit Bunch to Produce Biodiesel Production

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ABSTRACT

Every year, an empty fruit bunch (EFB) is extensively produced in Thailand, and this EFB has the potential to use it as the source of energy. A novel waste-to-energy technology of converting this agricultural waste into the value-added product has been studied. Microwave-assisted pyrolysis (MAP) is selected as the case studied. However, to extend the study of represent model of the biodiesel production plant, the development of the mathematical equation of this plant was performed with the aid of Design-Expert V.12.0.8 (trial) software. The distillate to feed ratio of the distillation column, the temperature of a heat exchanger, and the pressure of a decanter drum is selected as the independent variables for determining the product yield and utility cost. The result showed that the characteristic equations which can be used as a representative model for the yield of biodiesel, the yield of gasoline, and utility cost were significant with a 95% confidence level. The R-squared value predicted by the model was found to be 0.95-1.00. The mathematical model can be used for the analysis of product yield and the operating cost. The target of optimization has been set for maximizing product yields and minimizing the utility cost of the

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plant. The result showed that at the optimum operating conditions of the set of constraints e.g. distillate-to-feed ratio, the temperature, the pressure were 0.9, 60 C, 21.83 bar, respectively. At this optimum point, the values of biodiesel yield, gasoline yield, and utility cost are 5,909.45 kg/hr., 4,169.92 kg/hr., and 514.23 USD/hr., respectively.

INTRODUCTION

Nowadays, an empty fruit bunch (EFB) has been excessively produced in Thailand. According to the news report, the quantity of EFB produced in Thailand was around 34,114 tons in 2019. EFB has a potential as a source of energy to produce the precious product such as bio-oil. Many of research utilized fast pyrolysis to transform this agricultural residue into the bio-oil. But, recently, the novel technique of fast pyrolysis that it utilized the microwave substituting the fluidized bed is called Microwave-assisted pyrolysis (MAP). This technique has benefits for improved conversion efficiency of electrical power to heat, lower overall energy consumption, and a less complex stream of the pyrolytic products (1, 2). Therefore, this work developed the MAP process of EFB in Aspen Plus V.8.8 software. However, to extend the analysis of the model of the biodiesel production plant, the mathematical model is studied. Since the biodiesel plant has a purpose to generate biofuel production, some of the operating parameters will be investigated to maximize the yield of the product. In the case of mathematical development, this work utilized Design-Expert V.12.0.8 (trial) for designing the experiment and evaluation of the characteristic equation of the model.

Therefore, the objective of this work is to develop the fast pyrolysis plant, and the mathematical model of some independent parameters with the yield of the production plant. Developing this mathematical model can be used for optimization for maximizing the profit, and minimizing the utility cost.

MATERIALS AND METHODS

Process modelling

Table 1 Proximate and ultimate analysis of EFB (4)

Ultimate analysis	Air-dried (% wt.)
Carbon	43.80
Hydrogen	6.20
Oxygen	42.64
Nitrogen	0.44
Sulfur	0.09
Proximate analysis	
Moisture	8.34
Volatile	73.16
Ash	6.30
Fixed Carbon	12.20

Since the EFB is the raw material of this work, the elemental composition is presented in Table 1. The composition utilized in this study was cited from Kerdsuwan et al. (3). The base method of properties is selected for SOLIDS. The assumptions of the simulation were set up as follows: (a) The model is steady-state, (b) The model is isothermal and no pressure loss, (c) Most of the chemical device takes place at an equilibrium state, (d) All gases are ideal gases.

In the case of flow rate of EFB, it has been assumed for 28,000 kg/hr. For the operation process of the biodiesel production plant, the pretreatment is firstly required for modifying properties of EFB to be matched with the MAP mechanism. These pretreatment processes [A1] are drying and grinding. The purpose of drying is to remove the moisture content of the raw material since it possibly reduces the performance of the fast pyrolysis. But in the case of microwave implementation on fast pyrolysis, the moisture content will be acted as the microwave absorber that consequently improves the microwave heating mechanism (4). Hence, the appropriate range of moisture content should be reviewed. According to the work of Omar et al. (5), they have stated that the estimated proper moisture content was around 30% wt. for maximizing the microwave heating mechanism. Hence, this study selected the moisture content of EFB for 30%. Another pretreatment process is grinding. This step is to purposely reduce the size of the feedstock to enhance the pyrolysis mechanism. In the case of conventional fast pyrolysis, according to the review of Bridgwater (6), he has reported that the typical range of optimal size of EFB for fast pyrolysis is between 250 – 500 µm. In the case of MAP, Zhang et al. (7) has already summarized that the optimal particle size of any biomass feedstock that was reacted with the microwave-induced pyrolysis reaction should be roughly two times larger than the one that used for conventional pyrolysis. Hence, this work utilized the particle size for approximately 800 µm. When the pretreatment process has completely performed, pretreated EFB is then moved to the MAP process [A2] to transform into the value-added product, which is syn-gas, bio-oil, biochar. The kinetic reaction of fast pyrolysis of this study mostly cited from the research work of Peters et al. (8). These three products are mixed in a single stream and needed to be separated of each other in the separation section [A3]. Then, the cyclone will firstly separate the biochar of the pyrolyzed vapor. To separate the condensable vapor of incondensable vapor, this work utilized two flash drums condensate the bio-oil in vapor form. The by-products of this plant, the syngas, and biochar, were used for providing the heat inside the plant through the combustion process (A4). The main product of this work, bio-oil, will be further processed on the upgrading section to remove the impurities. The schematic of pretreatment, MAP, separation, combustion was shown in Figure 1.

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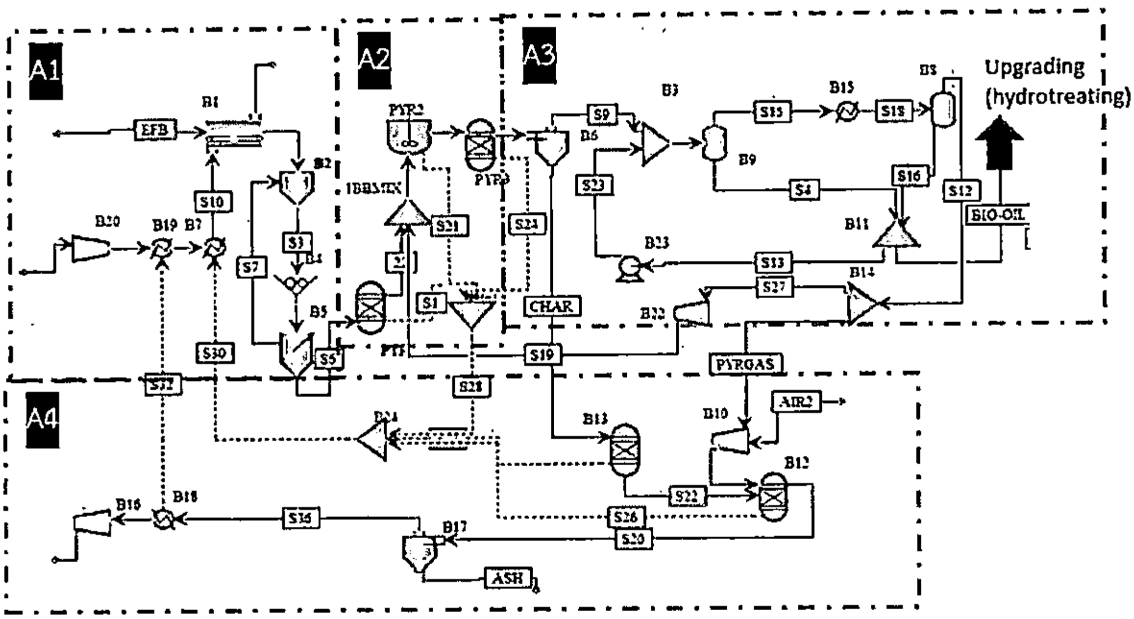

Figure 1 Pretreatment section [A1], MAP section [A2], Separation section [A3], Combustion section [A4] in Aspen Plus

For the upgrading section [A5], the hydrotreating process is performed in this sense. The hydrotreating required H_2 gases to react with bio-oil to pull out the impurities, which are basically oxygen and sulfur content. The required hydrogen consumption in this study was assumed for 0.05 g H_2 / g bio-oil (9). After the bio-oil has completely hydrotreated, this upgraded stream will be transferred to the distillation section [A6] to separate the gasoline and biodiesel production of each other. This study utilized two distillation columns to remove gasoline and biodiesel, respectively. The operating conditions of both gasoline and diesel columns have been shown in Table 2.

Apart from the precious products, the heavy stream, as a heavy residue of the distillation process, will be introduced into the hydrocracking process [A7] to performs the extraction of H_2 gases to recycle within the plant. The schematic of hydrotreating, distillation, and hydrocracking section that developed on Aspen Plus software was shown in Figure 2.

To summarize the operating conditions e.g. temperature and pressure, Table 3 has provided information on the main equipment throughout the plane.

Table 2 General information of distillation columns

Conditions	Gasoline col.	Diesel col.
Calculation type	Equilibrium	Equilibrium
Number of stages	9	8
Condenser	Partial-vapor-Liquid	Total
Reboiler	Kettle	Kettle
Reflux ratio (mass basis)	1.2	1.2
Distillate to feed ratio	0.51	0.45
The free water reflux ratio	0	0

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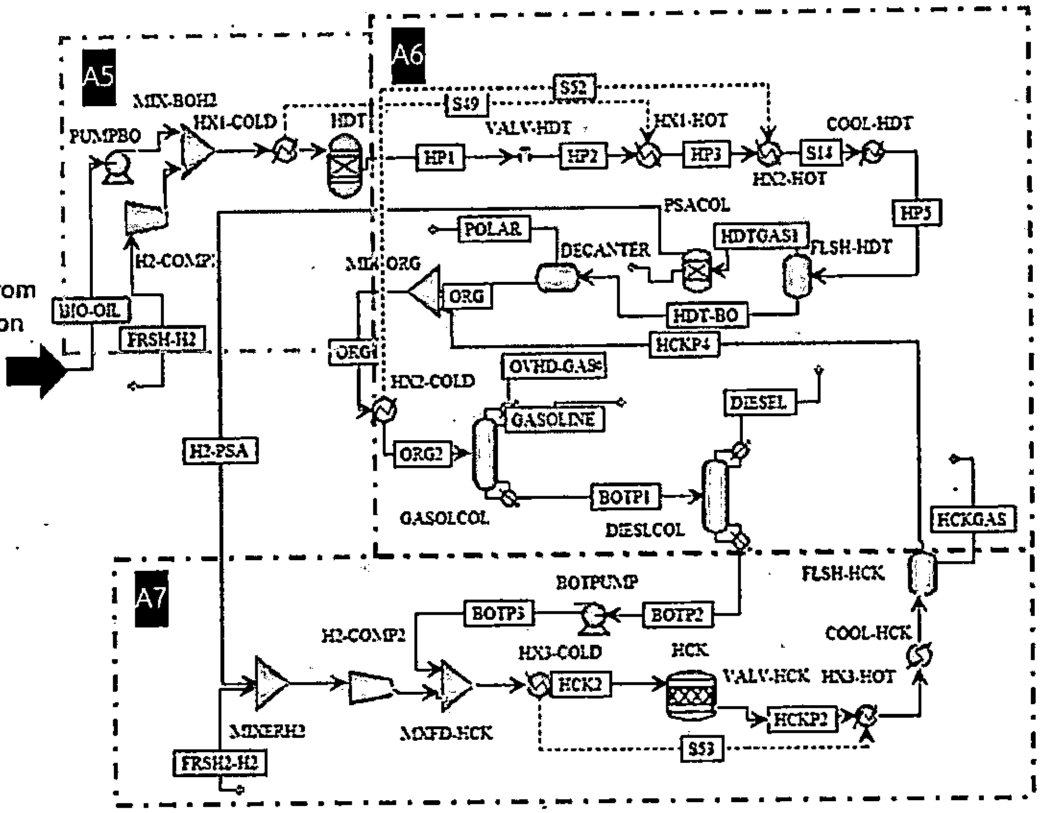

Figure 2 Hydrotreating section [A5], Distillation section [A6], Hydrocracking section [A7]

Table 3 Temperature and pressure in each equipment

Section	Equipment	Temperature/ Pressure
Pretreatment (A1)	B20 (compressor)	(-) / 1.2 bar
	B19, B7 (heat exchanger)	(-) / 1.2 bar
Fast pyrolysis (A2)	PYR1 (pyrolysis combustor, RYield) PYR2 (pyrolysis combustor, RCSTR) PYR3 (pyrolysis combustor, RYield)	500 °C / 1.2 bar
Separation (A3)	B9 (Flash drum, Flash2)	100 °C / 1.01325 bar
	B15 (heat exchanger)	250 °C / 1.01325 bar
	B8 (Flash drum, Flash2)	50 °C / 0 bar
Heat recovery (A4)	B10 (compressor)	(-) / 10 bar
	B13 (Ryield)	1,296 °C / 10 bar
	B12 (RGibbs)	1,296 °C / 10 bar
Hydrotreating (A5)	PUMPBO (compressor)	(-) / 87 bar
	H2-COMP (compressor)	(-) / 87 bar

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Section	Equipment	Temperature/ Pressure
	HX1-COLD (heat exchanger)	360 °C / 87 bar
	HDT (Ryield)	387 °C / 87 bar
Distillation (A6)	FLSH-HDT (flash drum, Flash2)	50 °C / 20 bar
	PSACOL (pressure swing adsorption, sep)	40 °C / 14 bar
Hydrocracking (A7)	BOTPUMP (compressor)	(-) / 90 bar
	H2-COMP (compressor)	(-) / 90 bar
	HX3-COLD (heat exchanger)	550 °C / 90 bar
	HCK (Rstoic)	677 °C / 90 bar
	COOL-HCK (heat exchanger)	50 °C / 1.01325 bar
	FLSH-HCK (Flash 2)	50 °C / 20 bar

Design of experiments

To achieve developing the process modeling, the experimental investigation should be performed for collecting the data as a result of the simulation. These data will be further used to develop the mathematical model of the biodiesel production plant. To developing the useful model, the suitable relationship between the independent variables and the response values is required. The objectives of this work are maximizing the product and minimizing the operating cost. Therefore, the yield of biodiesel, yield of gasoline, and utility cost are selected as the response values. In terms of the independent variables, the major parameters that significantly influence on the defined response were presented. In this sense, the distillation section is one of the most promising processes that directly influence the distinguish of gasoline and biodiesel out of the mixing stream. For the literature review, it has been founded that the main energy consumption shares a typical chemical plant accounting for around half of the total (10). To match the distillation column specification, the distillate to feed ratio of the column is selected as one of the variables. For the other two variables, this work selected the pressure of the flash drum (FLSH-HDT) and the temperature of the heat exchanger (COOL-HDT) as the independent variables. These two devices purposely remove the light hydrocarbons (C1-C4) and H_2 gas out of the hydrotreated stream. According to the study, these light hydrocarbons acted as the toxic compound in the bio-oil production (11). Apart from the independent factors, the other parameters were assumed to be a constant value.

After specifying the levels of independent factors, the levels were entered into the Design-Expert 12.0.8 (trial), and the experimental design matrix was given, as shown in Table 4. According to the methodology used 16 runs were obtained. Subtype was randomized. The design type was Central Composite Design (CCD).

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Table 4 The design matrix of the experiment

Run	Level of factors employed		
	A (-)	B (°C)	C (bar)
1	0.825	40	25
2	0.825	6.36414	25
3	0.9	20	15
4	0.825	40	25
5	0.698866	40	25
6	0.951134	40	25
7	0.825	40	8.18207
8	0.9	60	15
9	0.825	73.6359	25
10	0.825	40	41.8179
11	0.9	20	35
12	0.75	20	15
13	0.75	20	35
14	0.75	60	35
15	0.9	60	35
16	0.75	60	15

Where A is distillate to feed ratio of distillation of biodiesel in mass basis; B is the temperature of heat exchanger [COOL-HDT]; C is the pressure of flash drum [FLSH-HDT]

RESULTS AND DISCUSSIONS

The product composition of biodiesel and gasoline, as a result of simulating the Aspen Plus, has been shown in Table 5.

Table 5 Detailed compositions of the gasoline and the biodiesel obtained from the simulation.

Compositions	Mass fraction (%)	
	Gasoline	Diesel
WATER	1.32	0
CO_2	0.54	0
PROPANE	0.23	0
PROPENE	0.11	0
BUTANE	1.21	0
PHENOL	0.03	0.61
P-ISOPROPENYL-PHENOL	0	0.62
BENZENE	5.83	0
TOLUENE	1.64	0.02
M-XYLENE	0.77	0.82
ETHYLBENZENE	0.67	0.45
ISO-PROPYLBENZENE	0.42	3.87
PENTANE	3.04	0
N-HEXANE	6.11	0
N-HEPTAN	6.13	0.01
N-OCTANE	6.36	0.66
N-NONANE	0.91	5.29
MTYNONAN	0.13	5.03
UNDECAN	0.01	5.81
DODECAN	0	6.23
TRIDECAN	0	5.76
TETDECAN	0	5.97
PENTDECA	0	6.68
OCTDECAN	0	6.52
CYCLOPENTANE	5.58	0
CYCLOHEXENE	11.44	0
CYCLOHEXANE	15.76	0
METHYLCYCLOPENTANE	10.68	0
METHYLCYCLOHEXANE	12.07	0.06
N-PROPYLCYCLOHEXANE	0.85	11.9

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Compositions	Mass fraction (%)	
	Gasoline	Diesel
BICYCLOHEXYL	0	7.89
BICYCLOPROPYLHEXYL	0	7.02
NAPHTLEN	0	2.56
CHRYSENE	0	14.23
FURAN	1.97	0
DIMETHYLFURAN	4.32	0
ETHANOL	0.42	0
PROPANOL	0.44	0
BUTANOL	0.43	0
HEXANOL	0.02	0.28
PENTANOL	0.29	0.1
CYCLOHEXANOL	0.07	0.66

For the CCD, a total of 16 experimental runs of formulations was proposed by Design Experts software. It can be noticed that the run number 4 can be neglected because it has the same set of variables. Three factors are focused on, including the distillate to feed ratio of biodiesel column (A), the temperature of heat exchanger [COOL-HDT] (B), and the pressure of flash drums [FLSH-HDT] (C). The investigation then examined the various effects of the independent factors on the yield of biodiesel (kW), the yield of gasoline (kg/hr) and utility cost of this plant (USD/hr), to develop the characteristic model. The expected values for the plan of the experiment along with the recorded responses are presented in Table 6.

Table 6 Experimental matrix of CCD with defined response values

	Level of factors employed			Responses		
Run	A (-)	B (°C)	C (bar)	Y_1 (kg/hr)	Y_2 (kg/hr)	Y_3 (USD/hr)
1	0.825	40	25	5,904.42	4,145.34	528.07
2	0.825	6.36414	25	6,245.04	3,500.96	544.70
3	0.9	20	15	6,080.53	4,047.73	531.52
4	0.825	40	25	5,904.32	4,146.09	528.07
5	0.698866	40	25	5,441.36	4,675.33	533.06
6	0.951134	40	25	6,300.68	3,704.23	520.34
7	0.825	40	8.18207	5,486.66	4,771.30	524.32
8	0.9	60	15	5,756.67	4,372.41	512.88
9	0.825	73.6359	25	5,631.94	4,411.90	513.09
10	0.825	40	41.8179	6,179.30	3,548.35	530.51
11	0.9	20	35	6,533.09	3,089.74	536.98
12	0.75	20	15	5,587.27	4,614.40	535.15
13	0.75	20	35	5,999.73	3,727.11	539.75
14	0.75	60	35	5,647.82	4,352.32	520.09
15	0.9	60	35	6,148.76	3,774.51	516.58
16	0.75	60	15	5,288.15	4,893.06	516.66

Where A = Mass to distillate ratio of DIESELCOL, B = Temperature of COOL-HDT (°C), C = Pressure of FLSH-HDT (bar), Y_1 = Yield of biodiesel (kg/hr), Y_2 = Yield of gasoline (kg/hr), Y_3 = Utility cost (USD/hr

According to Table 6, the set of response will be used for developing the mathematical equation as a representative model of the system. The polynomial equations will be present as a relation between the varying parameters and the specified objectives of this study. The analysis of variance of the characteristic equation was performed. The results of the analysis are shown in Table 7. In this case, if the P-value of any independent variable is lower than the significance level of 0.05, it will be considered that the variable is significant with a confidence level of 95%. The model of the yield of biodiesel, yield of gasoline, and utility cost were found to be significant with a predicted R-Squared value of 0.9972, 0.9925, and 0.9595, respectively.

It can be noticed that all of these independent parameters, a distillate-to-feed ratio of a distillation column, the temperature of the heat exchanger, the pressure of flash drums, are significant with the proposed responses. For physical conditions of the heat exchanger and flash drums, are somewhat certainty relevant to the product yield and cost. Because these two independent parameters are the conditions that directly influencing the product composition as a result of changing its physical properties e.g. phase separation. But in the case of the distillate-to-feed ratio, its effect on the product composition might be not obvious. However, there is similar research that has experimented on the distillate-to-feed ratio on energy consumption in the separation device. They reported that this ratio was significantly impacted the product purity, as a result of the reflux rate of the condensed product at the overhead of the column (12).

Table 7 ANOVA of linear, quadratic and interactive terms of the biodiesel production plant on responses (P-value)

Sources	P-value of the responses		
	Yield of biodiesel	Yield of gasoline	Utility cost
Model	< 0.0001*	< 0.0001*	< 0.0001*
A-distillate-to-feed of distillation column	< 0.0001*	< 0.0001*	< 0.0001*
B-temp. of heat exchanger	< 0.0001*	< 0.0001*	< 0.0001*
C-pressure flash drum	< 0.0001*	< 0.0001*	0.0006*
A*B	0.1073	0.1949	-
A*C	0.0532	0.1278	-
B*C	0.0095*	< 0.0001*	-
A*A	0.0156*	0.0786	-
B*B	0.0135*	0.0003*	-
C*C	0.0004*	0.4240	-
R^2	0.9996	0.9990	0.9780

*significant

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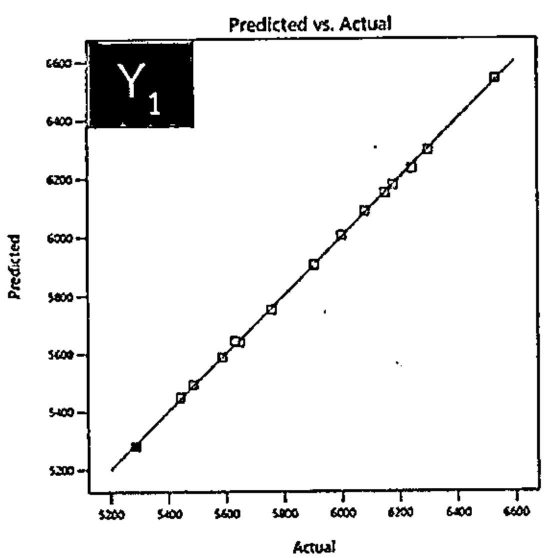
The model proposes the following polynomial equations for mass yield of biodiesel (Y_1), mass yield of gasoline (Y_2), and utility cost (Y_3), respectively:

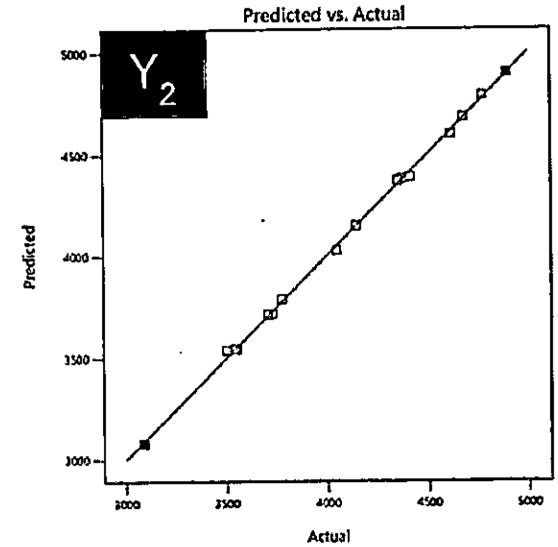
$$Y_1 = 1,468.27 + 6,685.77A - 5.48B + 25.81C - 4.76AB + 12.09AC - 0.08BC - 2,083.47A^2 + 0.03B^2 - 0.25C^2 \quad (1)$$

$$Y_2 = 9,966.04 - 8,884.09A + 7.25B - 40.60C + 8.8AB - 21.31AC + 0.44BC + 3,165.08A^2 - 0.16B^2 + 0.07C^2 \quad (2)$$

$$Y_3 = 569.28 - 34.25A - 0.48B + 0.20C \quad (3)$$

The linear graph plot of the responses, as a result of varying the variables, is shown in Figure 3. This figure signified the comparison between predicted and simulation value of mass yield of biodiesel, the mass yield of gasoline, and utility cost by graph Y_1, Y_2, Y_3, respectively. It can be observed that the developed linear correlation is fitted well with the actual value.





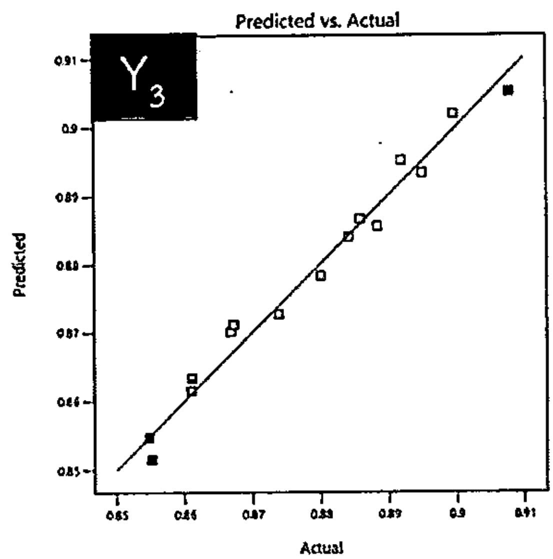


Figure 3 Linear correlation plot between the simulation and predicted response where Y_1 is the yield of biodiesel; Y_2 is the yield of gasoline; Y_3 is utility cost

For obtaining the optimal operating condition of interested independent parameters, the target of optimization has been set for acquiring the highest product yield and lowest utility cost. The optimum operating condition and outcomes have been presented in Table 8.

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Table 8 The optimal condition of the plant

Constraints (Independent factors)	Target (importance)	Optimal value
Independent factors		
Distillate-to-feed ratio	In range	0.9
The temperature (°C)	In range	60
The pressure (bars)	In range	21.83
Responses		
Biodiesel yield (kg/hr)	Maximize	5,909.45
Gasoline yield (kg/hr)	Maximize	4,169.92
Utility cost (USD/hr)	Minimize	514.23

CONCLUSION

This work focused on the effective utilization of agricultural waste, EFB in this case, to create some value-added bio-oil. The novel technology of fast pyrolysis where microwave heating is implemented was utilized. The developed mathematical model of the operating parameters in the distillation section with the objective of maximization of product and minimization of utility costs are also studied. The result showed the developed characteristic model indicated that the distillation process directly influences both of the yields of product and utility cost of this biodiesel production plant. The temperature and pressure, as conditions of the separation process, are certainty significant with the yield and cost, because of its capability of changing the phase of a product. For the distillation column, varying the distillate-to-feed ratio is recycling the condensed product, which has been undergone the distillation process, strongly related to the purity of the product, and subsequently the energy consumption of the column. These developed equations can be utilized for further analysis on the maximization of product and mitigation of operating cost.

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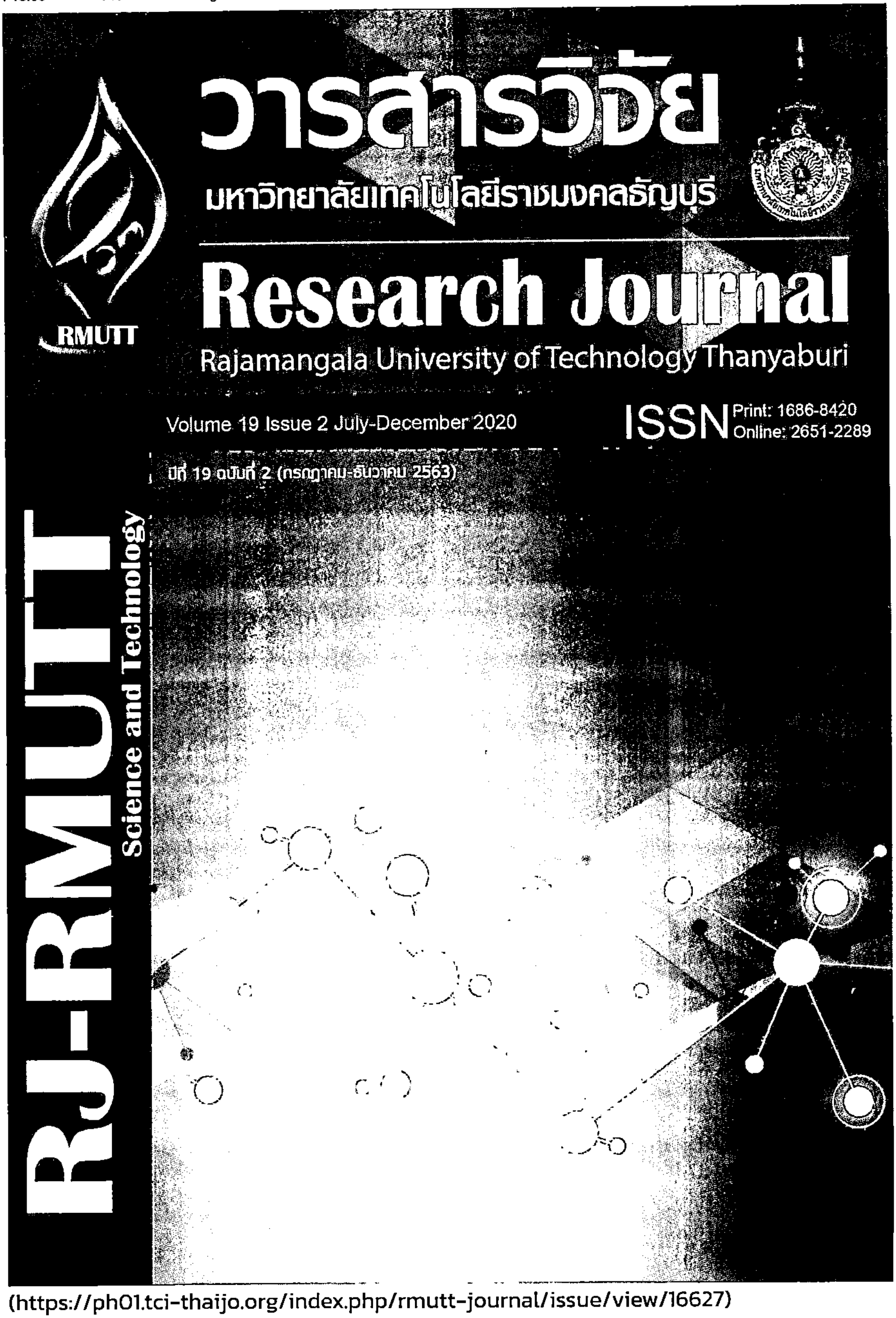

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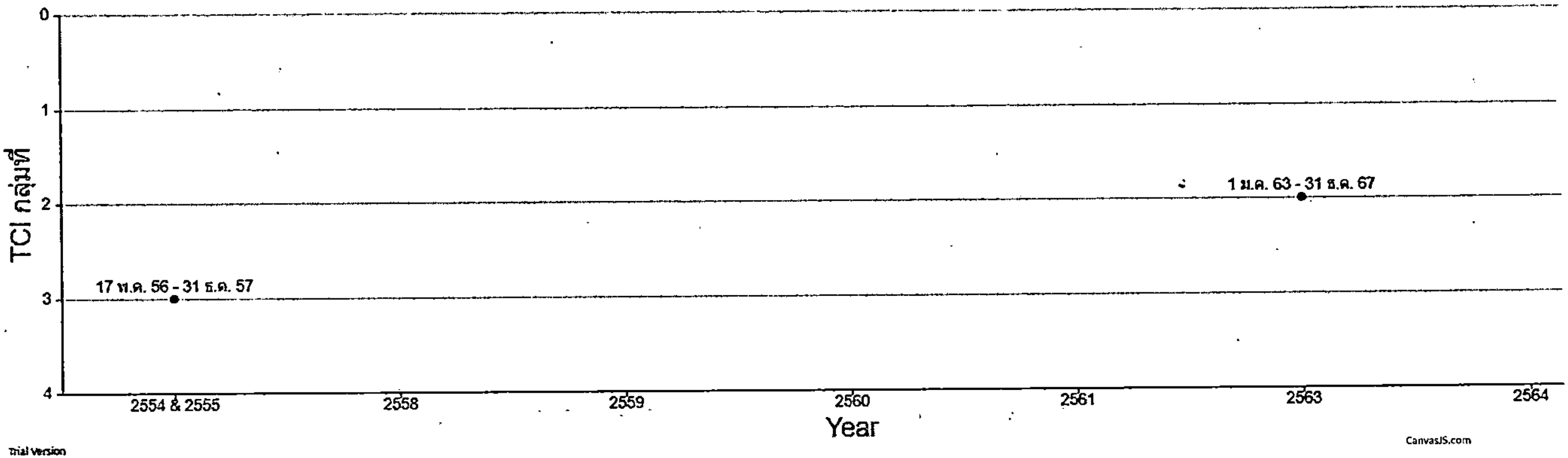

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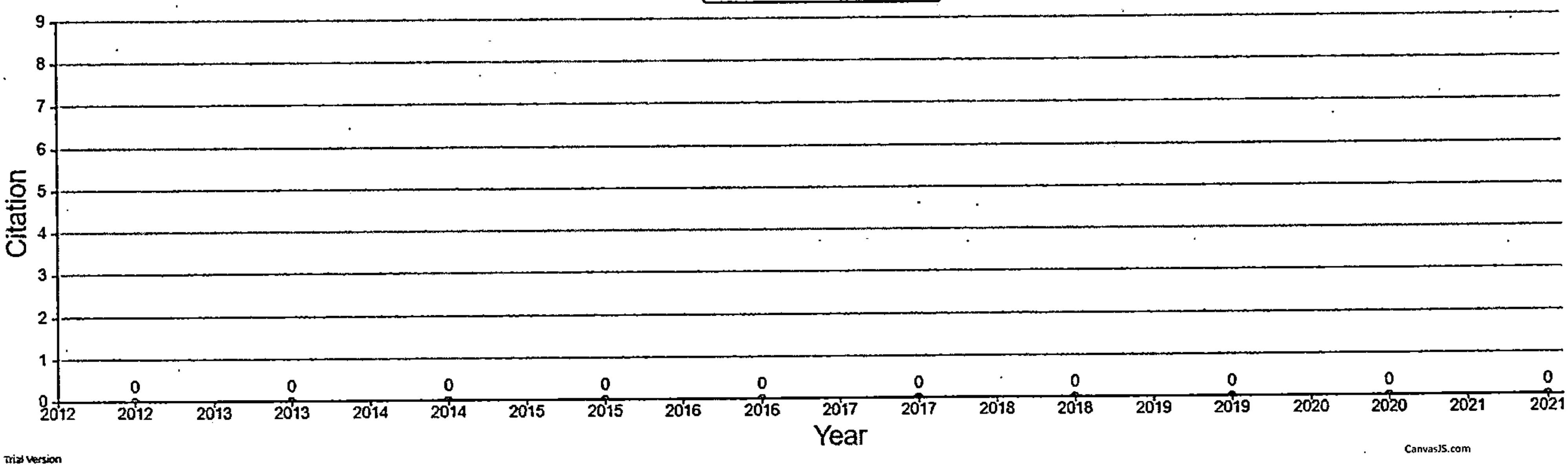

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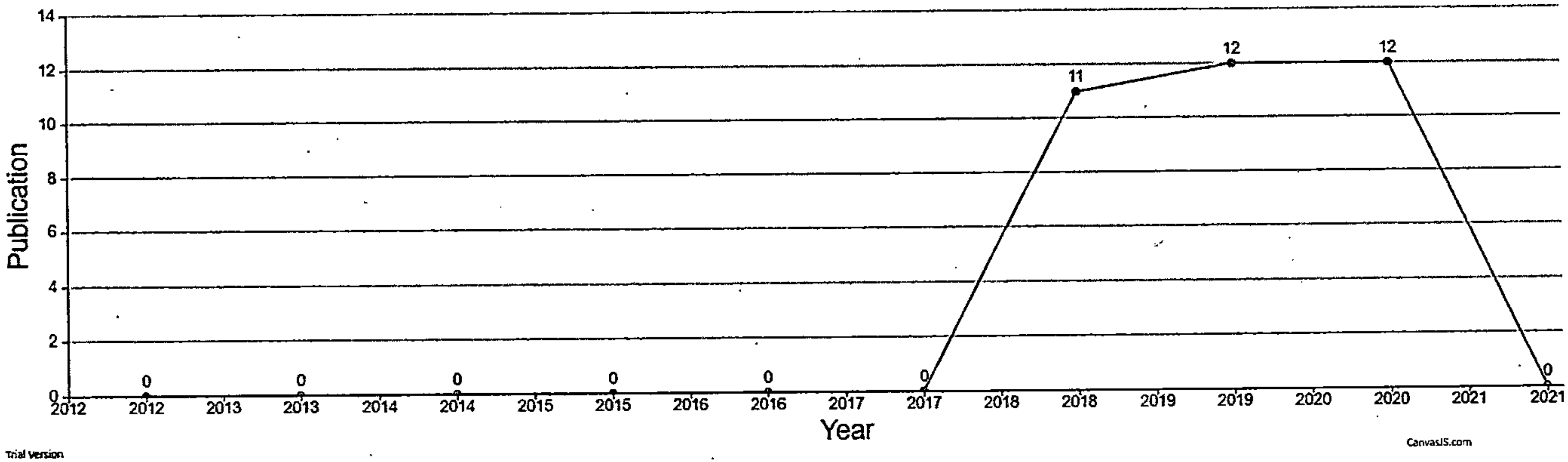

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