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An easy platform for calculating biodiesel yield with a graphical user interface

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ABSTRACT

An algorithm for calculating the biodiesel yield from esterification/transesterification was developed. The algorithm was represented in a program to facilitate researchers in exploring different types of feedstocks and catalysts. The input program of the preliminary yield data was processed numerically to generate reaction rate constant (k), reaction order (n), and activation energy (Ea) as a part of the kinetics response. The study revealed that the transesterification of used cooking oil and methanol with 0.25 wt% KOH catalyst had pseudo-first-order kinetics, with Ea = 21.7 kJ/mol. The optimum % yield obtained through the calculation was 96.5% at 323 K (50°C) within 10 h of reaction time. This program succeeded in validating secondary data from experimental research with a tolerance level of 10–17%. The program was validated where the model accuracy (R^2) for the first and second validations were 0.90 and 0.98, respectively. The application of this program is not limited to a specific biodiesel reaction design and can be extended to other designs as well.

Keywords: chemical kinetics computation; biodiesel yield; esterification; transesterification; graphical user interface

1. INTRODUCTION

The attention paid to non-fossil alternative fuels has been increasing, especially in developing countries. The Indonesian government, through the Ministry of Energy and Mineral Resources, utilizes biodiesel fuel, which is composed of fatty acid methyl ester (FAME) and a petrodiesel fuel mixture. The mandatory biodiesel program was implemented by the Indonesian government in 2018, with the issuance of Minister of Energy and Mineral Resources Regulation Number 32. The preliminary stage of biodiesel production used a blended content of 2.5%, consisting of 2.5% biodiesel and 97.5% diesel fuel. In 2010, the biodiesel content gradually increased to 7.5%. From 2011 to 2015, biodiesel content utilization increased from 10% to 15%. Furthermore, in 2016, the biodiesel content increased to 20%, popularly known as the B20 program. This progressed to the mandatory B30 program in 2020, and is now gradually moving towards B40 (Farobie & Hartulistiyoso, 2022).

Vegetable oil used as a feedstock for biodiesel comes from various sources. In Indonesia, FAME comes from oil palm plants, whereas in the Philippines (Obligado et al., 2017), it has come from coconut plants as coconut methyl ester (CME) since 2006. Furthermore, the United States (US) has considered and determined the use of oil from canola plants instead of soybean as feedstock for biodiesel (Biofuels International, 2022; Kell, 2023).

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Scientifically, fatty acids from vegetable oils of various sources have different types and amounts of carbon bonds. This fatty acid undergoes an esterification/ transesterification reaction that affects the physical and chemical properties of the biodiesel product. Researchers in India (Satyanarayana & Muraleedharan, 2011) have attempted to compare biodiesel from three different vegetable oil sources, where there were significant differences in the viscosity, calorific value, and cloud point properties of the resulting methyl ester (biodiesel). Meanwhile, several researchers in America and other areas (Martinez-Guerra & Gude, 2016; Lee et al., 2015) have tabulated the fatty acids chain from various oil feedstock as well as listing the physicochemical properties before and after they become methyl esters, where various yield or conversion percentage were obtained from those studies.

Several methods have been developed to optimize biodiesel yields. Researchers (Kaur & Ali, 2014; Srilatha et al., 2009) have successfully designed biodiesel experiments using heterogeneous catalysts and optimized them using kinetics equations. Other researchers (Gumahin et al., 2019; Kumar, 2020; Ogunkunle et al., 2017) have optimized the biodiesel reaction using non-kinetics methods, such as analysis of variance (ANOVA), central composite design (CCD), and artificial neural network (ANN), built using more than 10 data and tools that require sufficient memory. Therefore, studies related to the calculation and processing of biodiesel yield are still growing and relevant.

In this paper, a novel, simple program is reported based on our previous studies (Sofyan et al., 2021), which was built with three temperature and three reaction time variations to accommodate biodiesel experiments. This program can predict the optimum yield at a specific temperature and time. The program also provides a graphical user interface (GUI), which is easier to operate and read. It has also been reported in some studies (Torres et al., 2022; Morgado & Paiva, 2018; Ullah et al., 2021) that GUI-based programs are still open for various applications; hence, it is interesting to apply them to biodiesel fields. Various main reactants, including fatty acids, oils, alcohols, and catalysts, can be simulated using different parameters based on kinetics equations. This program can be used as an alternative for biodiesel researchers to observe the experimental phenomena of biodiesel.

2. MATERIALS AND METHODS

2.1 Computational method

Figure 1 shows a MATLAB flowchart that explains how the algorithm was designed (Oulasvirta et al., 2020). An experiment was designed based on the initial yield data for performing the calculation.

After the initial yield data was collected, the program was opened, and the data was input into the program interface. The data was then simulated by pressing the "s-curve" button. By pressing the button, the reaction rate constant (k), reaction order (n), and activation energy (Ea) before the smart-curve (s-curve) simulation model were calculated and displayed at the interface. At the end of the simulation process, the values of k, n, and Ea were displayed simultaneously with the appearance of the smart curve at the interface.

The optimum yield calculation was obtained by entering the reaction temperature input and the specific prediction time, subsequent to initial data collection. The program visualization is depicted in Figure 2.

2.2 Initial data collection (transesterification)

The feedstock (used cooking oil) was obtained from a restaurant in South Tangerang. The transesterification was conducted by reacting used cooking oil and methanol with a ratio of 1:2 (v/v) and adding KOH catalyst (0.25 wt% of oil) under continuous stirring. The process was carried out at various temperatures (40, 50, and 60°C) and times (6, 20, and 60 min). After the reaction was completed, the product was transferred into a separating funnel and left for a night until a biodiesel layer was identified. The transesterification result, in the form of biodiesel, was calculated using Equation 1:

$$\%\,Yield \;=\; \frac{W_B}{W_O}\, x\; 100 \tag{1}$$

where W_B = weight of biodiesel formed (g) and W_O = weight of used cooking oil used (g).

2.3 Yield determination by numerical method

An ideal yield (biodiesel conversion) was established under a certain time. The following formula was used to calculate the optimum yield:

$$Y = 1 - e^{-k\,t^{n}} \tag{2}$$

where Y = yield or the volume fraction of biodiesel conversion at a defined temperature (%), t = time (h), k = reaction rate constant (h^{-1}), and n = reaction order.

The ordinary differential equation with a numerical method was used as a solution to Equation (2), hence:

$$\frac{dY}{dt} = f(t, Y) = k - e^{-k\,t^{n}} \tag{3}$$

The use of natural logarithms is applied when assumed in the first order, and the reaction rate constant (k) is determined as follows:

$$Ln\,(1 - Y) = -k\,t \tag{4}$$

$$-\ln(1 - Y) = k\,t \tag{5}$$

The correlation coefficient, or R^2 (Equation 6), indicates the accuracy of the data. The correlation coefficient refers to the relationship or effect of the variables on the x- and y-axes of the trendline.

$$R^2 = \frac{\sum_{i=1}^{n}(y_{i-a_0-a_i x_i})^2}{\sum(y_i - \bar{y})} \tag{6}$$

The denominator displays the sum of the squares of the y component between the data and the model, whereas the numerator displays the sum of squares between the data and the model.

The three reaction temperatures were determined in order to create the biodiesel reaction model. Based on the Arrhenius equation (Equation 7), the reaction rate constant that was determined for each temperature was employed for the next phase, which involved creating a linear regression curve to ascertain the activation energy

(Ea) required for completing a two-hour conversion for each reaction temperature:

$$k = A\,e^{-\frac{E_a}{RT}} \tag{7}$$

where: k = as Equation 2 reaction rate constant (h^{-1}), Ea = activation energy (J/mol), R = ideal gas (8,314 J/mol K), T = reaction temperature (K), and A = collision factor or pre-exponential factor (constant).

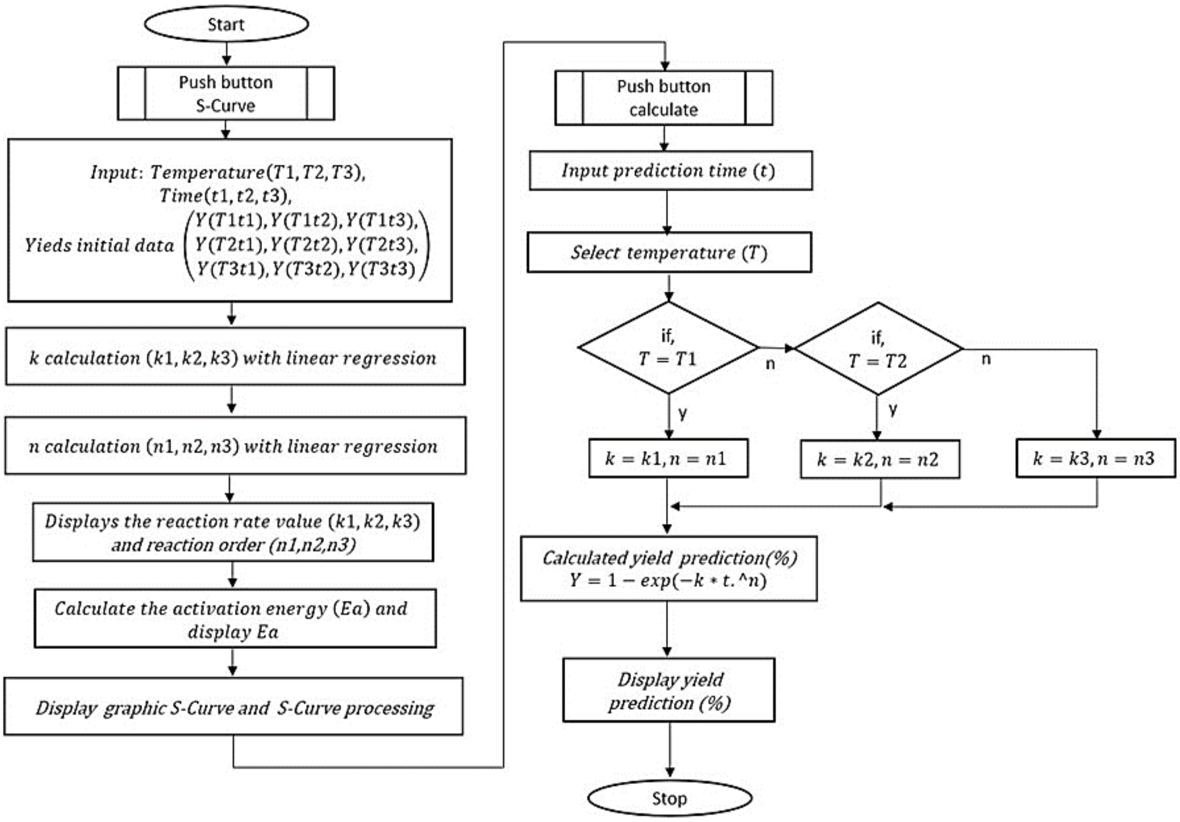
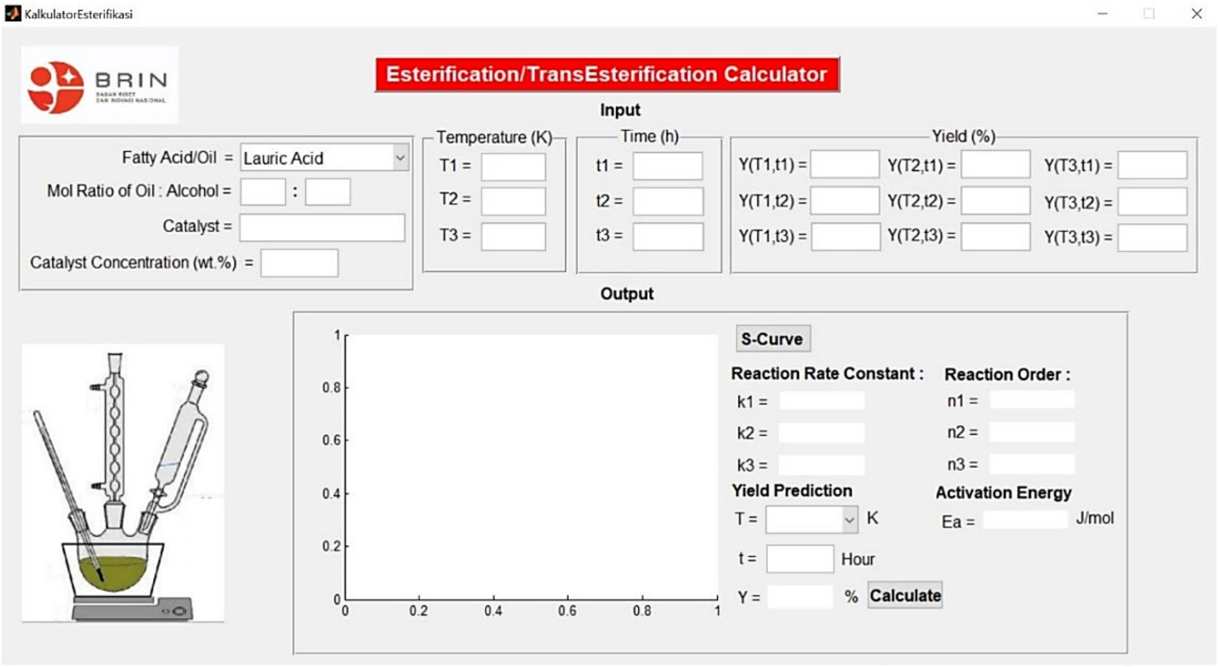


Figure 1. The program flowchart



Fatty Acid/Oil = Lauric Acid

Figure 2. The interface of esterification-transesterification program

2.4 Comparison and validation

This stage aimed to validate and compare the results of the program that has been developed with kinetics data obtained from similar literature. In this case, the developed program functions to calculate the value of the reaction rate constant (k), reaction order (n), and activation energy (Ea) in an esterification/transesterification reaction. The first step in this activity was to collect data from the relevant literature. The data were the same as those written in the interface program: type of fatty acid or oil, molar ratio, type of catalyst, concentrations of catalyst, temperature, time intervals, and initial yield. These data were used as a reference to compare the results obtained from the program.

Furthermore, the initial data were then entered into the program that had been developed. The program processed the data and generated k, n, and Ea values, which are important kinetics parameters in the reaction. The results obtained from the program were compared with the kinetics data obtained from the literature. In the comparison process, statistical analysis was applied to evaluate the extent to which the developed program is capable of producing results that are in accordance with the literature data. Several analytical methods were used, including regression analysis, calculation of relative errors, and hypothesis testing.

If the results obtained from the program are consistently similar to the literature data with an acceptable error rate, then it can be concluded that the program has been successful in estimating the reaction kinetics parameters. However, if there are significant differences between the program results and literature data, then the program needs to be evaluated further to improve its accuracy. The comparison-validation flowchart is shown in Figure 3.

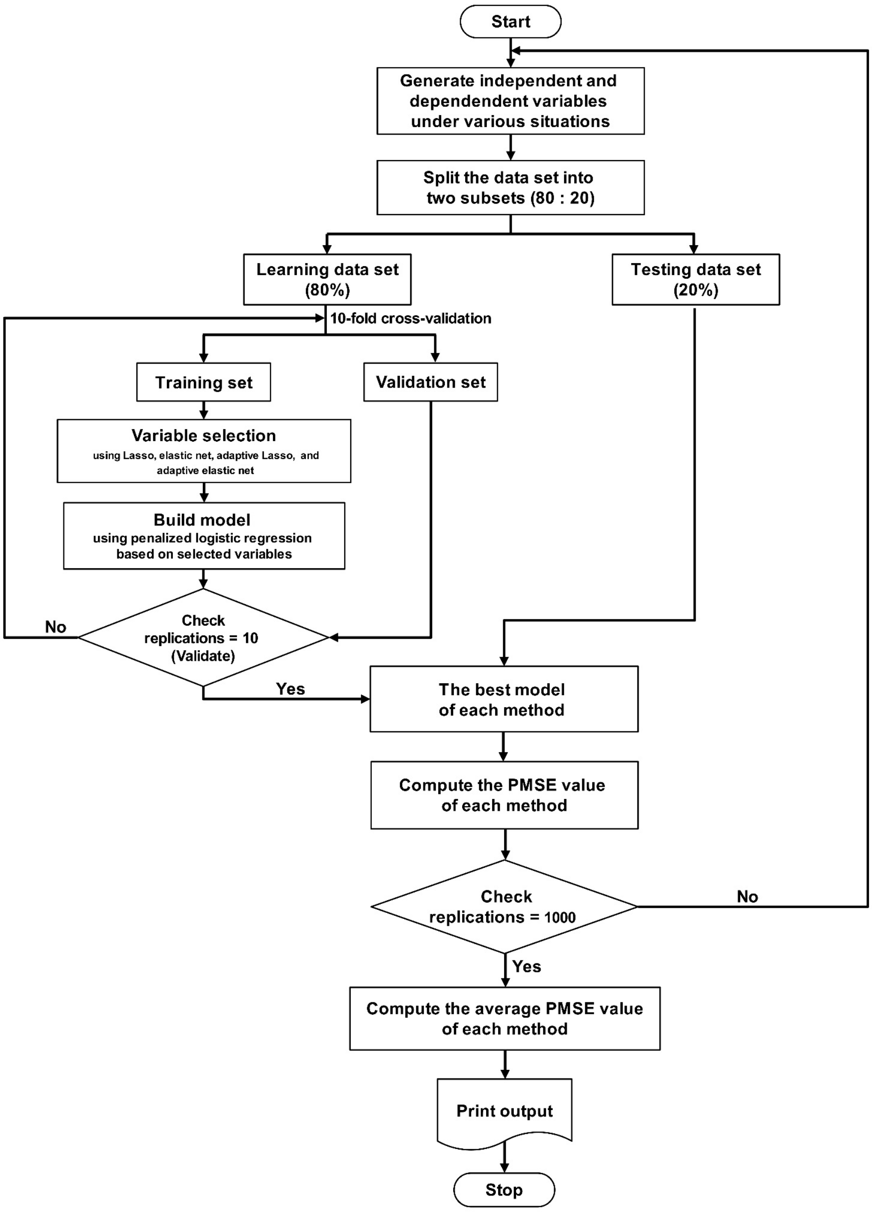


Figure 3. Comparison-validation flowchart

3. RESULTS AND DISCUSSION

3.1 Transesterification

Initial data on the yield of three temperature and three reaction time variations were successfully obtained from transesterification. According to the flow in Figure 1, the program performed numerical calculations to determine the value of k, n, and Ea before they were displayed on the program interface. The calculation results showed that the reaction was pseudo-first-order. This reaction order is also the same as other studies (Lukić et al., 2013; Stamenković et al., 2010; Vujicic et al., 2010) that experimentally calculated esterification reaction rate. The calculation results also showed that 21.7 kJ/mol was needed to start the biodiesel reaction.

Information was obtained from the s-curve plot, where T2 (323 K or 50°C) was the best reaction temperature among the three temperatures. For the same magnitude of reaction time, the calculations estimated that the yield obtained at T2 = 10 h was 96.5%. Meanwhile, the other yields obtained were only 79.3% and 93% at T1 and T3, respectively. The calculation results and the s-curve plot displayed on the program interface are represented in Table 1 and Figure 4, respectively.

3.2 Comparison and program validation

Secondary data were used as comparative literature on the esterification/transesterification of biodiesel. The data input into the program generated several outputs, which are summarized in Table 2. In a study by Srilatha et al. (2009), the experimental results of the esterification of palmitic acid and methanol with TPA/Nb_2O_5 catalysts showed that the reaction was successful in the pseudo-first-order. An increase in yield, which was directly proportional to the increase in temperature and reaction time, was also observed. The activation energy (Ea) was also identified as 63.2 kJ/mol. According to the s-curve (Figure 5a) and the calculation from the program, the result predicted that the reaction would gain 90% yield at 328 K (55°C) within 19.3 h.

Meanwhile, the experimental results of the transesterification of *Jatropha curcas* oil and methanol with Zr/CaO catalysts by Kaur and Ali (2014) showed that the reaction was also successful in the first order, as indicated by the average n value and the trend of the data. The value of Ea was 46.5 kJ/mol. Table 2 clearly shows that at 338 K, the yield process reached over 90% within 1 h. Hence, it is interesting to gain information on the yield at another temperature. According to the s-curve (Figure 5b) and the calculation from the program, the result predicted that the reaction would gain 90% yield at 308 K (35°C) and 318 K (45°C) when kept for 3.27 and 2.20 h, respectively.

A validation is presented in Table 3. In the first comparative data, information was not obtained about the reaction rate constant (k) value, whereas the activation energy (Ea) value obtained from our calculation only differed by 10% from the previous reports. For the second comparative data, there was a difference in the values of k and Ea by 17% and 9%, respectively. The difference in the value of k was probably due to the differences in the amount of data. Meanwhile, in the second validation, the Ea difference was better since it had a smaller percentage difference than in the first validation. Overall, these findings suggest that the calculation has a 10–17% difference compared with the literature data.

Finally, the experimental result and program data were analyzed using scattered graphs, as shown in Figure 6. In the first validation, the model accuracy (R^2) was 0.90, while in the second validation, R^2 was 0.98. From these two results, the program met the validation criteria. R^2 can be categorized based on its value, where a model is categorized as strong or has a good acceptance if $R^2 \geq 0.75$, as moderate if $0.5 \leq R^2 < 0.75$, and weak if $0.25 < R^2 < 0.5$ and $R^2 \leq 0.25$ (Hair et al., 2021).

Table 1. Program calculation (transesterification)

Abbreviation	Input				Output		
	Temp. (°C)	Temp. (K)	Time (h)	Yield (%)	k (h^{-1})	n	Ea (kJ/mol)
T1	45	318	0.1	20	0.27	0.77	21.7
			0.3	27.5			
			1	38			
T2	50	323	0.1	20	0.37	0.96	
			0.3	29.4			
			1	43.5			
T3	55	328	0.1	20.7	0.34	0.89	
			0.3	29.7			
			1	42.7			

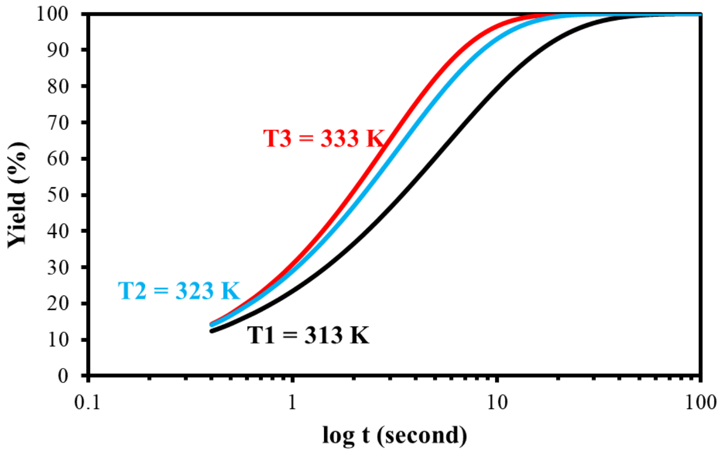


Figure 4. S-curve under different temperatures

Table 2. Program calculation from previous studies

Symbol	Input (secondary data)				Reference	Output program		
	Temp. (˚C)	Temp. (K)	Time (h)	Yield (%)		K (h^{-1})	n	Ea (kJ/mol)
T1	45	318	1	27.8	(Srilatha et al., 2009)	0.21	0.42	63.2
			2	42.8				
			3	52.8				
T2	50	323	1	31		0.38	0.56	
T2	50	323	2	57.3		0.38	0.56	
			3	68				
T3	55	328	1	35		0.44	0.56	
T3	55	328	2	62		0.44	0.56	
			3	73				
T1	35	308	0.5	30		0.67	1.05	
T1	35	308	1	42	(Kaur & Ali, 2014)	0.67	1.05	46.5
			1.5	64				
T2	45	318	0.5	39		0.98	1.09	
T2	45	318	1	67		0.98	1.09	
			1.5	77				
T3	65	338	0.5	75		3.22	1.20	
T3	65	338	1	95				
			1.5	99				

Table 3. Program validation

Parameter/response	1st validation		2nd validation	
	Srilatha et al. (2009)	Current study	Kaur and Ali (2014)	Current study
k (min^{-1})	-	0.01	0.06	0.05
Ea (kJ/mol)	57.2	63.2	42.5	46.5

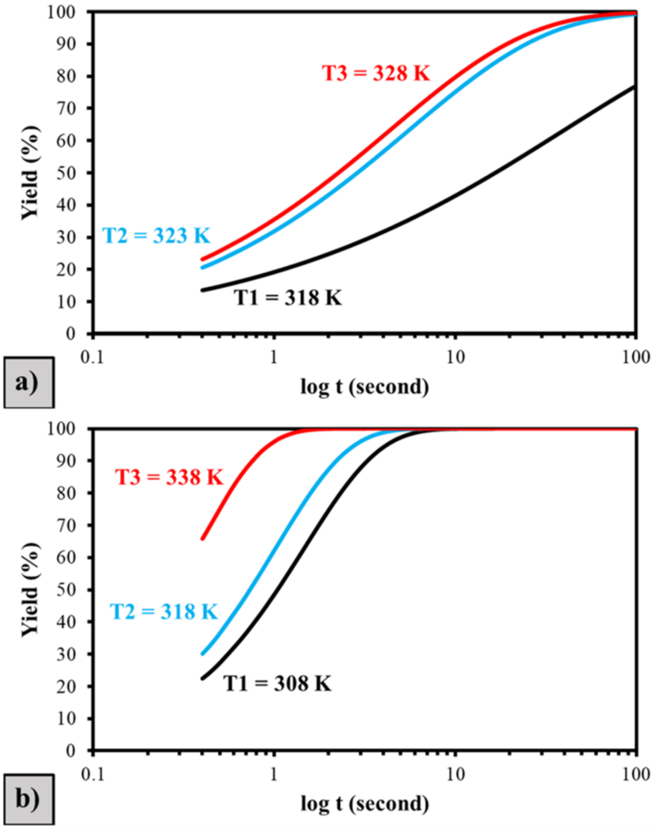


Figure 5. (a) S-curve of 1st comparative data and (b) the S-curve of 2nd comparative data with 3 replicates

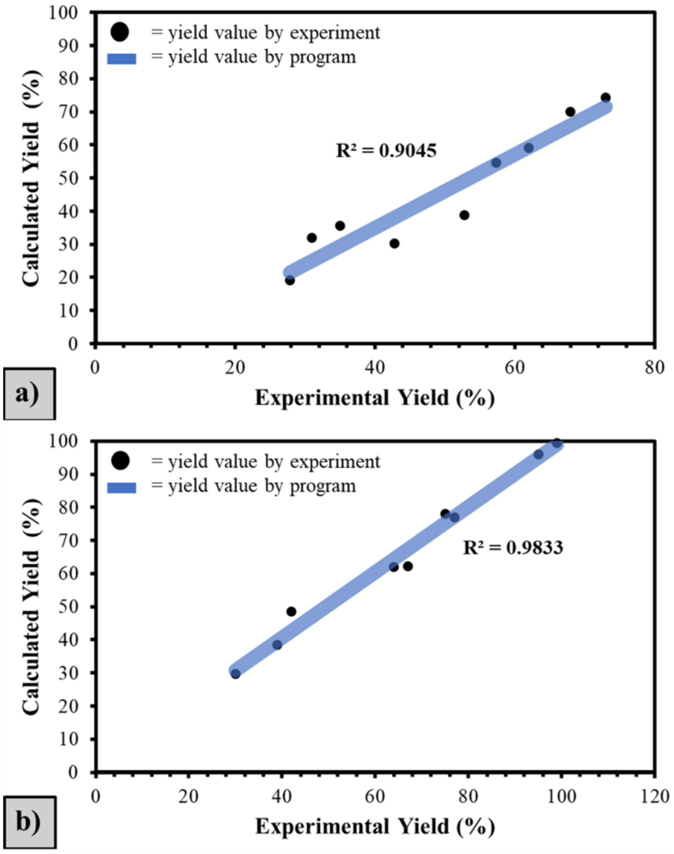


Figure 6. Experimental data vs calculated program for (a) 1st and (b) 2nd validations

4. CONCLUSION

A biodiesel calculator program with a graphical user interface was successfully built. The study revealed that transesterification of the used cooking oil and methanol with 0.25 wt% KOH catalyst had pseudo-first-order kinetics, with an Ea value of 21.7 kJ/mol, and the highest yield was reaching 96.5% at 323 K (50°C) within 10 h of reaction time. The program also effectively demonstrated that the esterification/transesterification can be applied with a tolerance of approximately 10–17%. After successful validation, the program acquired well-accepted model criteria based on a statistical analysis of model accuracy (R^2), making it applicable to other designs.

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