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Investigation of Fluid Flow in Biodiesel Reactor with 4 Different Types of Agitator using Computational Fluid Dynamics Simulation

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Abstract

Biodiesel is produced by transesterification reaction; animal or vegetable fatty acid reacts with the alcohol. Agitation of fluid in biodiesel production is required to develop the transesterification reaction in a biodiesel reactor. Agitation intends to decrease activation energy and increase the probability of collision between the materials. The objective of this research was to investigate fluid flow in a reactor with four kinds of agitators by using Computational Fluid Dynamics ANSYS FLUENT simulation and determine the optimum type of agitator in biodiesel production. The criteria of the agitation process which were studied include fraction and temperature distribution, turbulence, and fluid vorticity. The study used the helical screw, turbine, propeller, and anchor agitation types in transient and steady-state simulations. The material consisted of cooking oil and methanol with a mole ratio of 1:6 and used a rotational speed of 500 rpm with 60-65°C mixing temperature. The analytical hierarchy process method was used to decide the optimum agitator type. The result showed that the analytical hierarchy process score of each type of agitator was 0.314, 0.350, 0.249, and 0.087 for anchor, helical screw, propeller, and turbine agitator, respectively. Based on the analysis, the optimum agitator agreed on the helical screw type.

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1. Introduction

Biodiesel is an alternative fuel which renewable and environmentally friendly. Biodiesel is formed by a transesterification reaction (Figure 1) of triglycerides (vegetable or animal fatty acid) with alcohol (methanol) and produces Fatty Acid Methyl Ester (FAME)/biodiesel and glycerol (Ahmad *et al.* 2013; Alam and Tanveer 2020). In Indonesia, the vegetable oil type that has the potential to be used as raw materials for biodiesel production is palm oil.

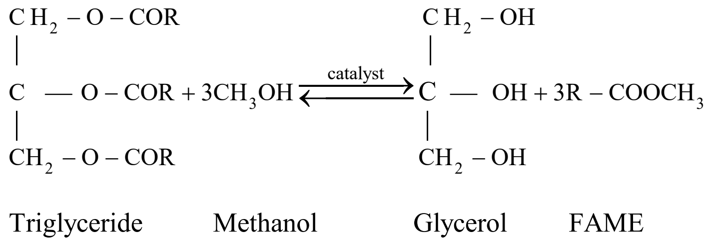

Figure 1. The reaction of biodiesel formation

Based on the study, the highest biodiesel concentration was achieved by following reaction conditions: temperature of 60°C, methanol to oil mole ratio of 6:1, catalyst concentration of 1%, and reaction time of 40-60 min (Lam and Lee 2011).

The cooking oil and methanol are immiscible (Satriana *et al.* 2012). Consequently, agitation is used to escalate the transesterification reaction effectively and increase the chance of collision between compounds. Forceful agitation will increase the diffusion of methanol in the oil considering to the mass transfer resistance is reduced (Budiman *et al.* 2021). The interaction of oil and alcohol during the transesterification reaction was complex. Hence, to obtain the complete intensity of functions determining the reaction, Computational Fluid Dynamics (CFD) simulation was used to analyze the reaction process's flow characteristic. The CFD method has advantages that it is more practical, the information obtained is not limited as in the experiment (only at the measurement point), and it can reduce the risk in the experimental method (Anderson 1995). This research aims to investigate the fluid characteristic in the biodiesel reactor and define the optimum agitator by observing the characteristic of temperature and fraction distribution, turbulence, and vorticity. Briefly, the uniformity of temperature and fraction distribution will increase the reaction process and increase the collision chance. Meanwhile, higher turbulence and vorticity will increase the agitation effect. Hence the reaction process in a biodiesel reactor will more effective. This aspect has a positive effect to yield numbers in biodiesel production. The agitators observed were anchor, helical screw, propeller, and turbine.

2. Materials and Methods

2.1 Physical Description

The fluid material used in the simulation consists of cooking oil and methanol. The physical and chemical properties of this material are shown in Table 1.

Table 1. Material properties of cooking oil and methanol

Material	Molecular weight (kg kmol^{-1})	Density (kg m^{-3})	Specific heat capacity (J kg^{-1}K^{-1})	Conductivity (W m^{-1}K)	Viscosity (kg m^{-1}s^{-1})
Cooking oil	860.76[a]	870.0[b]	1861[c]	0.170[c]	3.00×10^{-2} [b]
Methanol[d]	32.03	779.1	2550	0.198	5.09×10^{-4}

[a]Nitamiwati *et al.* (2018) [b]Sari *et al.* (2016) [c]Palm Oil proprties (2019) [d]ANSYS (2021b)

2.2 Model Geometry and Mesh

Biodiesel reactor simulation modeled existing reactor in Siswadhi Soepardjo Laboratory, Leuwikopo, Department of Mechanical and Biosystem Engineering, Faculty of Agricultural Engineering and Technology, IPB University. The agitator was modeled based on the design of Aubin and Xuereb (2006), McCabe *et al.* (2018), Jo *et al.* (2017), and Mezaki *et al.* (2000) for helical screw, turbine, anchor, and propeller agitator, respectively. Subsequently, model geometries then have been meshed to divide complex geometries into elements that could be used to discretize a domain. Model geometries and their mesh-generated result can be seen in Figure 2. In Figure 2, it can be seen that the reactor was installed with baffles and a heater. Baffles work to reduce the swirling in agitation. Hereinafter, the heater has functioned as a heat source. Geometries and mesh were generated by using tools in ANSYS 2021 R2 full version. The number of mesh and types applied in the reactor with different types of the agitator is shown in Table 2.

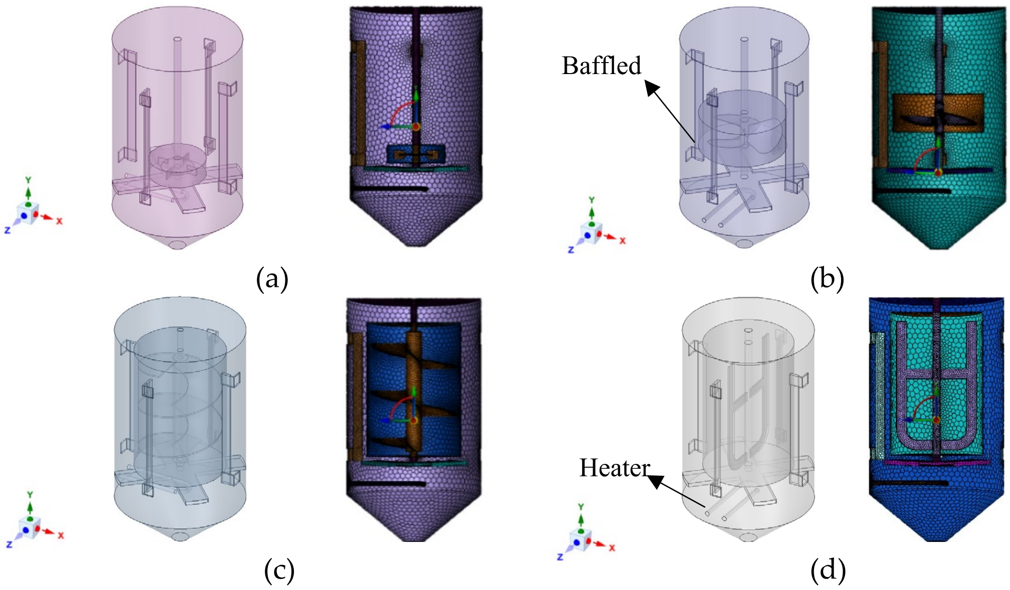

Figure 2. Fluid domain and meshing of biodiesel reactor with (a) turbine; (b) propeller; (c) helical screw; and (d) anchor

Table 2. Mesh type and number for each type of agitator

Agitator model	Type of mesh	Number of mesh
Turbine	Polyhedral	346,034
Propeller	Polyhedral	496,320
Helical screw	Polyhedral	459,795
Anchor	Polyhedral	418,350

2.3 Computational Fluid Dynamics Method

Computational fluid dynamics (CFD) is the rapidly evolving science of numerically solving the equations of fluid motion to produce a prediction and/or analysis of fluid flow phenomena by using computer-based numerical analysis and methods (Hu 2012). The phenomenon is modeled based on the law of conservation given as the following equations (ANSYS 2021a).

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = S_m \quad (1)$$

$$\frac{\partial}{\partial t}(\rho \vec{v}) + \nabla \cdot (\rho \vec{v}\vec{v}) = -\nabla p + \rho \vec{g} + \vec{F} \quad (2)$$

$$\frac{\partial}{\partial t}(\rho E) + \nabla \cdot (\vec{v}(\rho E + p)) = -\nabla \cdot \left(\sum_j h_j J_j \right) + S_h \quad (3)$$

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Equations 1, 2, and 3 are respectively known as law conservation of continuity, momentum, and energy. Expression ρ as fluid density (kg m^{-3}), t is time (s), $\vec{v}$ as velocity vector (m s^{-1}), S_m as source volumetric flowrate (kg m^{-3}s^{-1}), p as static pressure (Pa), $\vec{g}$ as gravity (m s^{-2}), $\vec{F}$ as force (N), E as activation energy (J), h enthalpy (J kg^{-1}), J as mass flux (kg m^{-2}), and S_h as volumetric flowrate from another source (W m^{-3}).

2.4 Boundary Condition and Simulation Setup

Biodiesel reactor simulation used ANSYS Fluent 2021 R2. The simulation used material properties, as shown in Table 1. It also used cooking oil and a methanol mole ratio of 1:6. Analysis type used transient and steady-state simulation. The transient simulation was conducted for 15 minutes, assuming the fluid flow was steady. The domain was divided into two domains, namely the stationary domain, and the rotating domain. The rotating domain described the rotating state of the agitator with an angular velocity of 500 rpm. The detail setup describe in Table 3.

Table 3. Set up and boundary condition

Description	**Parameter**	**Input**	**Value**
General	Solver type	Pressure-based	-
	Solver time	- Transient	15 minute
		- Steady	-
	Gravity	Active	g (y^- direction)
Model	Multiphase	Mixture model	-
	Energy	On	-
	Viscous	Realizable, k-epsilon	-
Domain	- Stationary	-	-
	- Rotating	Frame motion	500 rpm
Reactor wall, baffle, blade	Wall	Heat Flux	0 W/m^2
Heater	Wall	Temperature	65^{o}C
Solution method	Pressure-velocity	SIMPLE	-
	Pressure	PRESTO!	-
	Momentum	First order upwind	-
	Energy	First order upwind	-
Initial	Oil	High (*y-axis*)	0-252 mm
		Temperature	60^{o}C
	Methanol	High (*y-axis*)	252-305 mm
		Temperature	30^{o}C

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2.5 Determining Optimum Agitator

Analysis for determining the optimum agitator was carried out based on the simulation result. It was done by analyzing temperature and fraction distribution, flow turbulence, and vorticity. Further, the optimum agitator type been judged using the Analytical Hierarchy Process (AHP) method.

2.5.1 Temperature and fraction distribution. This analysis was conducted to observe the uniformity by examining the standard deviation of temperature and fraction distribution, using equation 4 and considering the ratio of its minimum to maximum value using equation 5.

$$S = \sqrt{\frac{\sum_{i=1}^{n}(x_i - \bar{x})^2}{n-1}} \quad (4)$$

$$k = \frac{x_{\min}}{x_{\max}} \times 100\% \quad (5)$$

In equations 4 and 5, S is the standard deviation, x_i is the value of the sample items, $\bar{x}$ is the mean value, n stands for the size of the sample, and k is the uniformity in percent (%) by calculating the ratio of minimum value (x_{min}) and maximum value (x_{max}). In the mixing process, it was expected temperature and fraction to be evenly distributed. The S value approach showed it to 0 or the k value approach to 100%.

2.5.2 Flow turbulence**.** In this research, turbulence was analyzed by viewing the turbulence intensity. It is defined as the ratio of the velocity fluctuation and its average velocity and mathematically, formulated as the following equations (ANSYS 2021a).

$$I = \frac{u'}{\bar{u}} \times 100\% \quad (6)$$

$$u' = \sqrt{\frac{1}{3}(u_x'^2 + u_y'^2 + u_z'^2)} \quad (7)$$

In equations 6 and 7, the I expresses turbulence intensity in percent (%), $ú$ is the root-mean-square of velocity fluctuation (m/s), $\bar{u}$ is the average velocity (m/s), and $ú_x$, $ú_y$, $ú_z$ are velocity fluctuation (m/s) in the direction of x, y, and z, respectively.

2.5.3 Vorticity**.** It represents the local and random circular motion of a particle in a fluid flow. Vorticity (ζ) value, mathematically formulated by equations below (Cengel and Cimbala 2006).

$$\xi = \nabla \times \vec{V} \quad (8)$$

$$\xi = \left(\frac{\partial w}{\partial y} - \frac{\partial v}{\partial z}\right)i + \left(\frac{\partial u}{\partial z} - \frac{\partial w}{\partial x}\right)j + \left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}\right)k \quad (9)$$

The vorticity value (1/s) is the result of the vector product of the velocity derivation values with each axis x, y, and z. This axis represents cartesian coordinates, while u, v, and w describe each velocity in the x, y, and z-direction.

2.5.4 Analytical Hierarchy Process (AHP) method. Agitator type selection was conducted by comparing the criteria and alternatives. In the AHP method, the first step was determining the goal, which was the selection of the optimum agitator. Then determined the criteria and alternatives choices. The criteria had been judged by experts, while the alternative had been rated based on the simulation result. Furthermore, in pairwise comparison, the level of importance of one criterion/alternative was compared to another. From the AHP method, the final weight of each alternative agitator was obtained. The optimum agitator was the agitator that had the highest final weight.

3. Results and Discussion

3.1 Characteristics and Flow Behaviour in Biodiesel Reactor

The characteristics and behavior of fluid flow in the biodiesel reactor were observed to investigate the motion of the fluid in the reactor. The fluid flow formed by each agitator had different characteristics. The range of values can be seen at legend for each agitator in simulation result Figure 3. It shows the velocity contour inside the biodiesel reactor with varying types of agitators in vertical and horizontal plan view. Figures 3 (c) and (d) depict that fluid velocity in the agitation process was only high around the agitator blades. In general, it can be seen that slow velocity occurred at the bottom of the biodiesel reactor. High velocity occured around the blade due to the rotational effect and direction of rotation of the agitator. Meanwhile, in the bottom of reactor got a slight agitation impact.

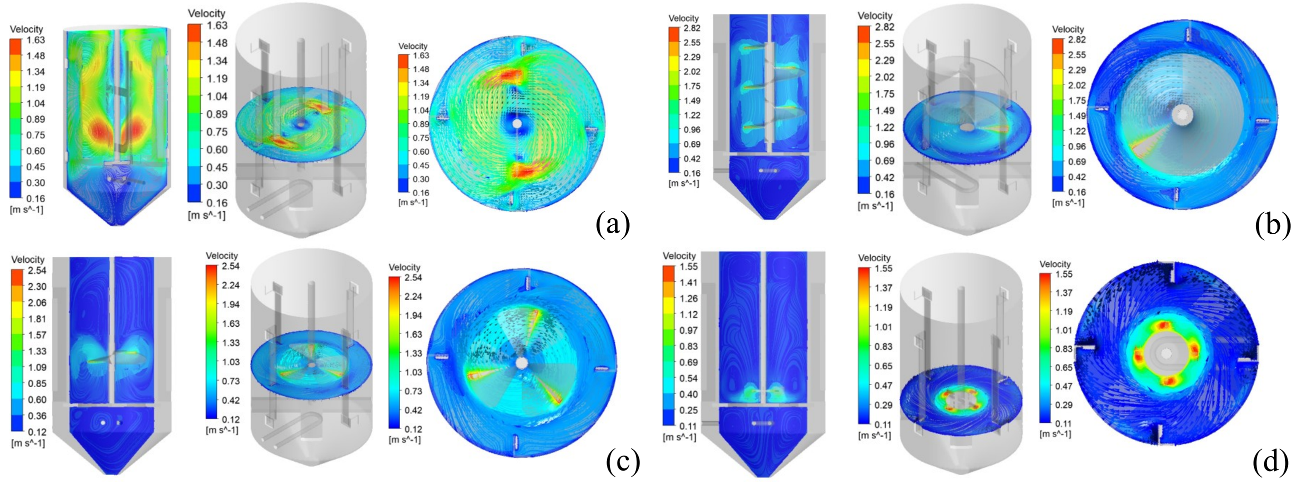

Figure 3. Fluid flow with agitator type of (a) anchor; (b) helical screw; (c) propeller; and (d) turbine

3.2 Methanol Fraction Distribution

Methanol fraction distribution was observed to identify the presence of methanol inside the biodiesel reactor. The cooking oil and methanol present in the same area could indicate the possibility of collisions between the materials. The chemical reaction in transesterification occurs when the reactant particles collide with each other (Suarsa 2017).

The CFD simulation results of fraction distribution are shown in Figure 4. Figure 4 (a) describes the methanol fraction distribution in the biodiesel reactor using an anchor agitator. Fraction values range from 0 to 1. The value of 0 shows the absence of methanol in a particular area, while the value of 1 indicates the entire presence of methanol in a specific area. The figure shows that the methanol fraction distribution began to be uniform at 10 minutes. Figure 4 (b) represents the biodiesel reactor using the helical screw agitator. Visually, uniformity was achieved lower than in the first minute. The application of the propeller type of agitator is shown in Figure 4 (c). The uniformity also was reached during the first-minute agitation process. Figure 4 (d) represents the agitation process using turbine type. It can be seen that the uniformity of the methanol fraction was not achieved even though it's been 15 minutes agitation process. Comprehensively, all type of agitators had methanol fraction when it reaches steady condition was 0.20.

Using equations 4 and 5, the standard deviation and uniformity of methanol distribution were then quantified. The results are shown in Figure 5. The mixing process using the helical screw type of agitator, methanol distribution more quickly to achieve uniformity. In the standard deviation graph in Figure 5 (a), the value toward 0 represents a more even mixture. While the diagram in Figure 5 (b), the value closer to 100% indicates a more even mixing. After the helical screw agitator, the mixing process achieved a more even distribution of methanol fraction using propeller, anchors, and finally turbine type of agitator, sequentially. Figure 5 also explains that during the 15 minutes mixing process with the turbine agitator, the distribution of the methanol fraction was relatively uneven. This can be seen from the rather significant standard deviation value and the percentage of uniformity which was still below 10%, while mixing with other agitators the uniformity had reached above 80%. This can also be seen visually in Figure 4.

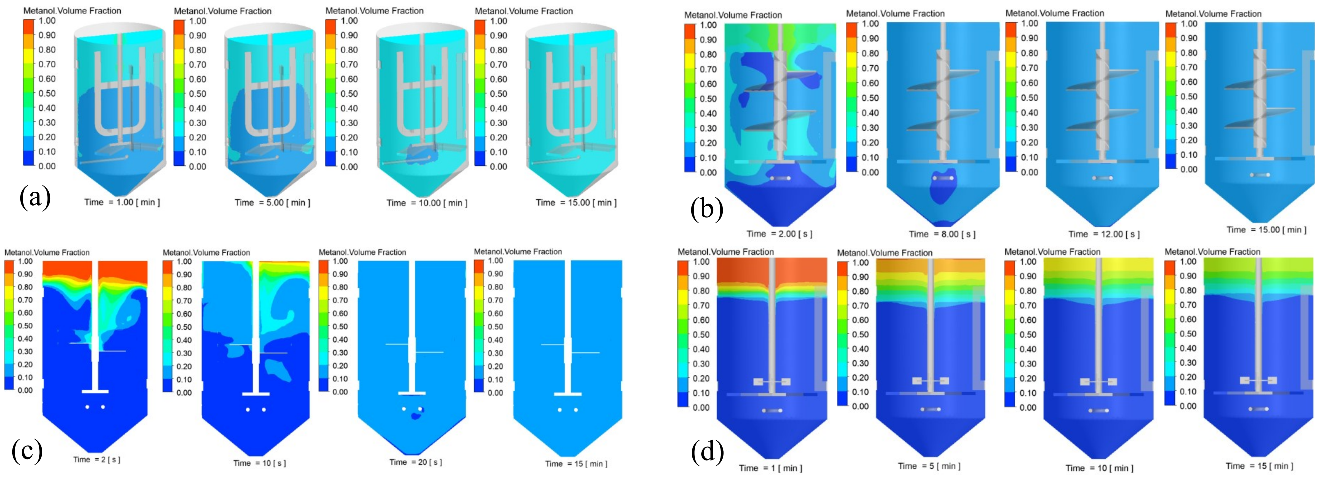

Figure 4. Methanol fraction distribution used (a) anchor; (b) helical screw; (c) propeller; and (d) turbine

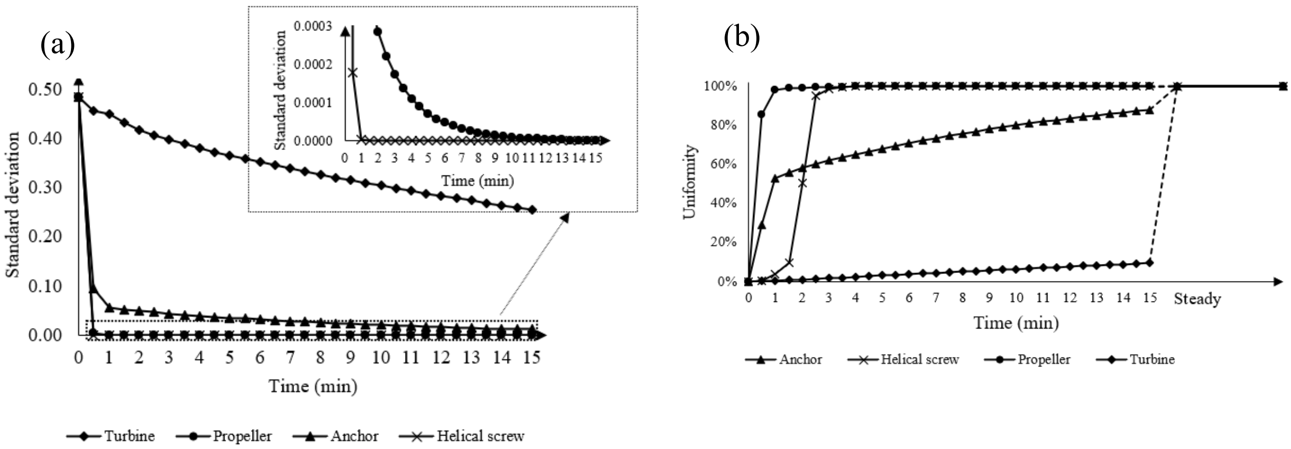

Figure 5. Value of (a) standard deviation and (b) uniformity in methanol fraction distribution

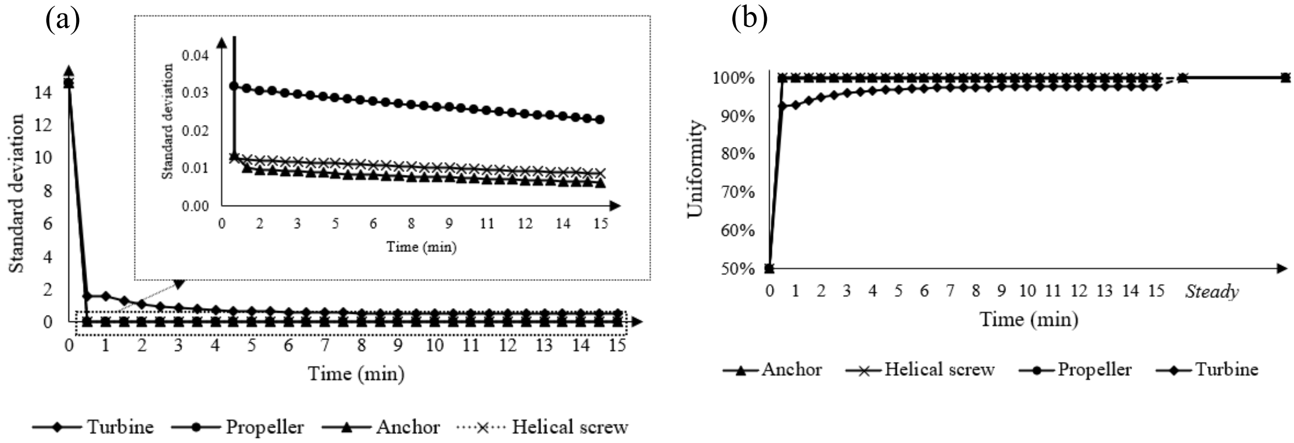

Figure 6. Value of (a) standard deviation and (b) uniformity in temperature distribution

3.3 Temperature Distribution

The CFD simulation result shows that the uniformity in the biodiesel reactor was above 90% in 15 minutes of the mixing process. Figure 6 defines the standard deviation and uniformity of temperature distribution. Figure 6 shows that temperature distribution in the biodiesel reactor was relatively homogeneous (>90%). The agitation process using the turbine type produced lower temperature uniformity than others. It can be seen in Figures 6 (a) and (b).

3.4 Flow Turbulence

The turbulence that occurred in the reactor was expressed in terms of turbulence intensity. The results of the CFD simulation's intensity of this turbulence can be seen in Figure 7. It shows that the agitator type that produced the highest turbulence was the anchor type. The most elevated turbulence could increase the mixing effect in the reactor.

3.5 Vorticity

Based on the simulation result, the vorticity value for each agitator type can be seen in Figure 8. It indicates that the anchor type was the highest vorticity value in the agitation process. It interprets this agitator could produce a local vortex of fluid in the tank higher than other agitators. The presence of flow vortices will cause the laminar flow layer in the area near the wall to decrease due to the formation of turbulence which can increase convective transfer (Kaci *et al.* 2010).

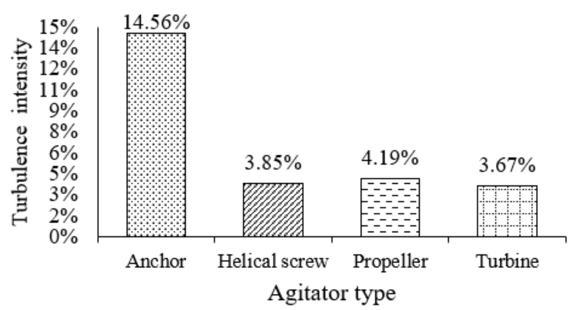

Figure 7. Turbulence intensity for each agitator

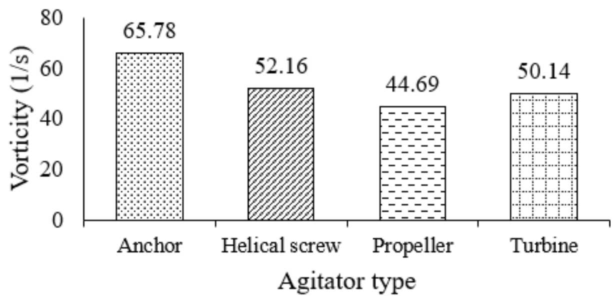

Figure 8. Vorticity value for each type of agitator

3.6 Agitator Selection

Referring to the simulation result obtained, an assessment was conducted by comparing the criteria and alternatives. These values were processed using the Analytical Hierarchy Process (AHP) method thus the final score of each agitator was determined. The agitator with the highest score was then selected as the optimum agitator. Experts' judgment did criteria assessment by giving value to the questionnaire. Meanwhile, the alternatives were rated based on the CFD simulation result. The assessment result for the criteria is shown in Table 4.

Table 4. The weighting of each criterion

Criterion	Weight
Temperature distribution	0.054
Fraction distribution	0.595
Vorticity	0.233
Turbulence	0.118

Table 4 explains that fraction distribution had the highest weight. For the continuity of the reaction between methanol and cooking oil, the main point was that the agitation could spread the materials evenly so that oil and methanol collide and the chemical reaction process could occur. If the material "piled up" in a certain area, the reaction would not occur. For vorticity and turbulence, the agitator was designed to be able to create a turbulent (not laminar) flow to increase the chance of collisions between materials. The bigger the collision, the higher the chemical reaction between the particles, because the contact between the surfaces of two or more materials would frequently occur and the activation energy for the reaction would be more minor. Meanwhile, the temperature distribution was in the last order, because the materials used were a liquid phase in the reactor so the heat would propagate faster. In other words, the temperature distribution would be evenly distributed as long as the mixed fluid moved and the heat transfer occurred only by convection.

Furthermore, Table 5 shows that the helical screw type had the highest final score, which means this agitator was selected as the optimum agitator for the mixing process in a biodiesel reactor. When observed for each criterion, the anchor type of agitator had the higher weight for the criterion of temperature distribution, vorticity, and turbulence. The helical screw type had the highest importance on the methanol fraction distribution criterion. However, at the final score, it can be seen that the helical screw type had the highest value because the fraction distribution criterion had the highest score compared to other criteria.

Table 5. The weighting of each alternative

Alternative	Criterion				Final score
	Temperature ditribution	Fraction distribution	Vorticity	Turbulence	
Anchor	0.455	0.181	0.519	0.515	0.314
Helical screw	0.320	0.455	0.201	0.131	0.350
Propeller	0.181	0.320	0.079	0.262	0.249
Turbine	0.045	0.045	0.201	0.092	0.087

4. Conclusion

The study of fluid flow in the reactor was carried out using various agitators, namely anchor, helical screw, propeller, and turbine types. The assessment was done by using the AHP method resulted in an importance score for each criterion, which was 0.054 (temperature distribution), 0.595 (methanol fraction distribution), 0.233 (vorticity), and 0.118 (turbulence). From these results, it can be seen that the methanol fraction distribution criteria had a more important role than other criteria. Meanwhile, the final score for each type of agitator were 0.314 (anchor), 0.350 (helical screw), 0.249 (propeller), and 0.087 (turbine). Then the helical screw type was chosen as the optimum agitator for the biodiesel reactor because it had the highest score value. The study was conducted in a simulation. Therefore, it was suggested to experiment to compare the quality and yield of biodiesel produced.

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