Simulation of biodiesel production using perforated helical type static mixer

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Abstract. The main objective of this simulation was to estimate fluid characteristics due to the presence of holes in the perforated helical type static mixer using Computational Fluid Dynamic (CFD) during the process of biodiesel production with static mixing reactor. The conventional helix compared to the perforated helix with three scenarios of holes, namely with one hole each side of the helix as 1st scenario, two holes each side of the helix as 2nd scenario and three holes each side of the helix as 3rd scenario. Simulated CFD of biodiesel production showed the mixing process with the help of perforated helical type static mixers provided a better mixing impact compared to conventional helix. The concentration of fatty acid methyl ester (FAME) using perforated helical type (as much as 86.26%) was higher than conventional helical type (as much as 82.79%). In other word the number of FAME concentration was increased by 4.06% due to the presence of perforated helix. While, the viscosity was decreased by 15.33%.

1. Introduction

Biodiesel is a fuel-based mono-alkyl ester which main component comes from new/used vegetable oils and animal fats [1]. The characteristic resemblance to diesel oil causes biodiesel has great potential as an alternative fuel [2]. In addition, biodiesel also more environmentally friendly due to the emissions produced in the form of carbon neutral, low sulfur [3], carbon monoxide and unburned hydrocarbons, furthermore it has lower generated solid particle emissions than diesel fuel [4]. Biodiesel production (also known as trans-esterification) divided by catalytic and non-catalytic process. These process are distinguished by the involvement of the catalyst during the reaction. Catalytic process using base catalyst [5] and acid catalyst [6] to reduce activation energy, non-catalytic process using supercritical methanol vapour [7] and superheated methanol vapour [8] to increase kinetic energy of reactant particles. However, the increase in kinetic energy is done by using a very high temperature (superheated methanol vapour) and also high pressure (supercritical methanol vapour) which is very risky for an explosion. Accordingly, the catalytic production process still the most widely used because not only the reaction time tends to be faster than other processes but also easier to be applied. Whatever the method is, one of the most critical factor in each method is the collision frequency between reactant particles. The higher the frequency the more likely the trans-esterification reaction will succeed.

One way to increase the collision frequency other than increasing temperature and pressure is by increasing the mixing intensity. Conventional mixing processes such as blade agitator can generate
vortex [9] and this method also involves moving parts that is very risky for leakage during the stirring process. Especially when it’s done at high temperature, because alcohol is flammable. Therefore, it’s very crucial to find a method that can carry out stirring purpose without involving moving parts, for example by utilizing a static mixer system. Static mixer system is a common method and already widely used in the chemical industry to create a more homogeneity mixture. In the static mixing system, the fluid flows continuously through the static elements as if experiencing stirring in the tank conventionally. There are many types of static mixers, but the most widely used for biodiesel production is the helix one especially using base catalyst [10][11][12][13]. The geometry of helical type allows the mixing results more homogeneous after going through division and reversal of the flow. The kinetic energy formed by the flow [14] leads to the formation of smaller particles, as a result the surface area becomes larger and increases the collision frequency.

In addition to the conventional helical type static mixer, a perforated helical type also has potential for biodiesel production process. The perforated helical type is a conventional helical type with a perforated surface [15]. This shape is considered able to increase the abilities and the mixing results of a conventional helical type static mixer because the holes will create a better flow division [16]. However, the use of perforated helical type for biodiesel production especially in a continuous system has never been done yet. Therefore, it is necessary to do a simulation to see the flow division and patterns that occur in the reactor. By doing this it can be seen whether the mixing process is better or not for biodiesel production in the future. This research will discuss flow patterns and results that can be achieved in the catalytic biodiesel production process by using several perforated helical type scenarios.

2. Materials and methods
This simulation performed using Computer with RAM 8GB and with the help of CFD simulation in Ansys Fluent 19.2. Ansys fluent is a computational fluid dynamic software that used to model flow for industrial application. With the help of Ansys fluent, the fluid movement in the reactor can be predicted by using boundary conditions from the actual data. The characteristics of the materials can be seen in Table 1.

| Fluid parameter | Triglyceride | Methanol | FAME | Glyceride |
|-----------------|--------------|----------|------|-----------|
| Molecular weight (g mol\(^{-1}\)) | 858\(^{[11]}\) | 32 | 287\(^{[11]}\) | 92 |
| Density (kg m\(^{-3}\)) | 870\(^{[13]}\) | 785 | 850\(^{[18]}\) | 1259.9 |
| Dynamic viscosity (kg m\(^{-1}\) s\(^{-1}\)) | 0.0300933\(^{[13]}\) | 0.0005495 | 0.001955\(^{[18]}\) | 0.799 |
| Heat capacity (kJ kg\(^{-1}\) C\(^{-1}\)) | 1902\(^{[17]}\) | 2534 | 1112\(^{[13]}\) | 2427 |
| Conductivity (W m\(^{-1}\) C\(^{-1}\)) | 0.1708\(^{[17]}\) | 0.2022 | 0.1705\(^{[17]}\) | 0.286 |

| Geometry parameter |  |
|---------------------|---|
| Tube diameter (m)   | 0.0254 |
| Tube length (m)     | 0.66 |
| Twist angle (degree)| 180 |
| Helix length (m)    | 0.04 |
| Helix width (m)     | 0.0254 |
| Helix thickness (m) | 0.001 |
| Perforated diameter (m) | 0.004 |
| Perforated spacing (m) | 0.005 |
| Number of elements  | 12 |

Other parameters that being used were reaction temperature (65°C), materials flow rate (9 l.min\(^{-1}\) for triglyceride and 2 l.min\(^{-1}\) for methanol) [13]. Before starting the simulation, the activation energy and collision factor could be determined using Arrhenius equation, see Equation (1).
where: \( k = \text{reaction rate constant}; \) \( T = \text{temperature (Kelvin)}; \) \( R = \text{the gas constant (J K}^{-1} \text{ mol}^{-1}); \) \( E_A = \text{activation energy (kJ mol}^{-1}); \) \( A = \text{collision factor (mol}^{-1}). \) Arrhenius equation could also be stated in logarithmic form, see Equation (2).

\[
\ln k = \ln A - \frac{E_A}{RT}
\]

There were two liquid materials that used in this simulation. These materials would be forming a mixture liquid, so the viscosity and density value of the mixture material could be determined by using Equation (3), (4), (5), and (6).

\[
m_{f1} = \frac{n_1}{n_{ttl}}
\]

\[
m_{f2} = \frac{n_2}{n_{ttl}}
\]

\[
\vartheta_{camp} = m_{f1}\vartheta_1 + m_{f2}\vartheta_2
\]

\[
\rho_{camp} = m_{f1}\rho_1 + m_{f2}\rho_2
\]

Where, \( m_{f1} = \text{mole fraction of triglyceride}; \) \( m_{f2} = \text{mole fraction of methanol}; \) \( n_{a} = n_1 + n_2; \) \( n_1 \) and \( n_2 = \text{mole of methanol and mole of} \) \( \text{triglyceride (mole)}; \) \( \vartheta = \text{mixture viscosity (kg m}^{-1} \text{ s}^{-1}); \) \( \vartheta_1 = \text{viscosity of} \) \( \text{triglyceride (kg m}^{-1} \text{ s}^{-1}); \) \( \vartheta_2 = \text{viscosity of methanol (kg m}^{-1} \text{ s}^{-1}); \) \( \rho_m = \text{mixture density (kg m}^{-3}); \) \( \rho_1 = \text{density of} \) \( \text{triglyceride (kg m}^{-3}); \) \( \rho_2 = \text{density of methanol (kg m}^{-3}). \)

The velocity of fluid in a pipe could be determined using Equation (7)

\[
v = \frac{Re \vartheta}{D}
\]

To get the three-dimensional flow pattern, the Navier-Stokes equation was used, see Equation (7) [19]:

\[
\rho \frac{\partial u}{\partial t} - \nabla \cdot (\rho u (u + (\nabla u)^T)) + \rho (u \cdot \nabla) u + \nabla p = 0
\]

Where: \( \nabla \cdot u = 0; \) \( \vartheta = \text{dynamic viscosity, u = vector velocity, } \rho = \text{fluid density, and } p = \text{pressure} \)

The law of conservation of momentum in a static mixer can be calculated by Equation (9):

\[
\frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho uu) = \nabla p + \nabla \cdot (\tau) + F
\]

Where: \( \tau \) is the stress tensor and \( F \) is the external body forces.

The geometry for the helical type elements for all models were built using 3D-CAD from Auto CAD 2019 application and Design Modeller from Ansys Fluent 19.2 then simulated using CFD simulations from Ansys Fluent 19.2. The static mixer that being examined was a helical type with three scenarios. Conventional helical type static mixers (Figure 1a) was used for a validation purpose. Validation was done by comparing the simulation results (using conventional helical type) with the experiment data. All boundary condition that being used in simulation were came from the experiment data. All scenarios can be seen in Figure 1. The first scenario (Figure 1b) was a helical type static mixer with two holes (one hole on each side of helix), the second scenario (Figure 1c) has 4 holes (two
holes arranged perpendicular to the axis on each side of helix), the third scenario (Figure 1d) has 6 holes (three holes arranged in a triangle form on each side of helix). Each hole was made in a diameter of 0.004 m. The number of mixer elements were 12 elements for each reactor and the number of reactors were five with 0.66 m of length [13]. After designing geometry, meshing process, entering boundary conditions, initializing and calculating then the CFD simulation can be performed. Each scenario was inside 5 reactors that arranged as in Figure 2.

![Figure 1](image1.png)  ![Figure 2](image2.png)

**Figure 1.** Geometric of the helix type static mixer in the reactor; (a) conventional (without holes), (b) 1<sup>st</sup> scenario, (c) 2<sup>nd</sup> scenario, (d) 3<sup>rd</sup> scenario.  
**Figure 2.** Full geometry with 5 reactors

The results obtained from simulation were compared with the experiment data by using Equation (10):

\[
\text{Error (\%)} = \frac{|\text{Experiment} - \text{simulation}|}{\text{Experiment}} \times 100\%
\]  

(10)

### 3. Results and discussion

Simulation of using perforated helical type static mixer for biodiesel production was done after determining and validating the results and the boundary conditions using conventional helix type. If the results indicated that it could represent real conditions, then all boundaries condition would be used for simulation using the three scenarios.

#### 3.1. Validation of model

The validation process carried out for this research was using conventional helical type static mixer. The simulation results obtained were compared with the actual data that using static mixer with the same type, same geometry and number of elements in one reactor. The parameter to be compared was the percentage of FAME produced from 1<sup>st</sup>, 3<sup>rd</sup> and 5<sup>th</sup> reactor. The experiment data was obtained by doing an experiment using five reactors that filled with 12 elements of helical static mixer [13]. The relationship between simulation and experiment data can be seen in Figure 3.

![Figure 3](image3.png)  
**Figure 3.** Validation using FAME concentration (%)
Error percentage (using Equation 10) of FAME concentrations got from CFD simulation were about 8.07%, then all boundaries or operation condition that being used for conventional helical type static mixers would be used on the perforated type too to predict the flow in reactor. Thus, the results obtained in each scenarios could be compared.

3.2. Simulation using perforated helical type

From the Figure 3 can be seen that the simulation results were close to the actual data even though there was still deviation. This was because the simulations were built using equations or real condition approaches.

3.2.1. Velocity. Velocity is an important factor in the reaction process between reactants. By increasing the speed, the mixing and the particle collision will be even greater. Thus, the number of particles that can react to produce FAME will also increase. From Figure 4 can be seen the velocity vector that took place in each reactor. Reactor with conventional helix static mixers had a lighter vector colour intensity than others. The other three scenarios had almost the same colour level. For more details, you can see in Figure 5.

![Figure 4. Velocity vector: (a) conventional helix; (b) 1st scenario; (c) 2nd scenario; (d) 3rd scenario](image)

![Figure 5. Closer Velocity vector view: (a) conventional helix; (b) 1st scenario; (c) 2nd scenario; (d) 3rd scenario](image)

Increased speed in all three scenarios compared to conventional helix due to the presence of holes. When the fluid flows through the reactor, in addition to experiencing the process of flow distribution, mixing and stirring as the main function of the helix type mixer, some fluid also flew through the
holes on the helix surface so that when they collided with other fluid particles the mixing process got better. The third scenario had higher FAME concentration than the others. This is because there were a greater number of holes so the mixing process got better.

From Figure 5 can be seen that the mixing process that occurred in all helix models produced a different pattern. The results from perforated helix showed a more intense mixing. This can be seen in the area around the holes with an intense colour. The colour indicated that the velocity in this section was high and this also illustrated that the collision also high. The increased speed could also affect the increased in the number of fluid particles that had the opportunity to react due to interactions caused by collision factors between particles.

3.2.2. Visosity. Viscosity is one of the parameters that shows the quality of a biodiesel. One of the purpose of trans-esterification of triglycerides with methanol is to reduce the viscosity of the material. Because the high viscosity will give an incomplete combustion effect on the combustion engine and the appearance of crust in the fuel sprinkle that will reduce the motors age.

![Figure 6. Viscosity from CFD simulation](image_url)

From Figure 6 it is clear that the simulation result from all helix models had an almost equal viscosity. The existence of a helix type static mixer had a very large impact on the first reactor and begins to slow down from the third and fifth reactors. This could occur because the value had almost reached a stable value for biodiesel viscosity.

Reactors on the three scenarios had almost the same effect on the viscosity (i.e. 0.0052617 Pas for the first scenario, 0.005127 Pas for the second scenario, and 0.00497 Pas for the third scenario). The decrease in viscosity from the simulation of three scenarios were much greater when compared to the conventional helix model (0.00586958 Pas) especially in the third scenario which was smaller by 15.33% than conventional helix. This show the influence of holes in the mixer element that could improve the stirring and mixing process that occurred during the reaction as a result the mixture becomes more homogeneous.

3.2.3. Biodiesel concentration. Biodiesel concentration in this project is the number of fatty acid methyl ester (FAME) that produced during reaction in every end/ outlet of reactor. The effect of the holes on the mixer elements can be seen in Figure 7.
From Figure 7 can be seen that the FAME concentration in all static mixer model had increased dramatically from the first reactor to the third reactor (82.79% for conventional helix, 85.71% for the first scenario, 86.08% for the second scenario and 86.16% for the third scenario). This shows the effect of stirring and mixing on the static mixer had a very big effect, especially after entering the first static mixing reactor. The increase of the FAME concentration due to stirring and mixing could be clearly seen at the beginning of the reaction, but it slowed down after going through the third and fifth reactors. This show that the value had almost reached the maximum value that could be achieved from the reaction or had almost reached the end of the reaction. Figure 7 also shows that in the third scenario, the FAME concentration was slightly higher compared to the conventional type (by 4.06%). This proved that there was an influence of holes in the helical type static mixer to increase the FAME concentration. As seen in Figure 4 there was an effect of holes on the speed of materials passing through the mixer elements.

The existence of holes on the helix increased the speed of colliding fluid particles because some of the fluid that was supposed to experience resistance and impact on the helix surfaces, passed through the holes and when it came out the holes it collided with other particles at different speeds thereby increasing the mixing process that occurs. This had an effect on the increasing number of particles that can react which is marked by the increasing FAME concentration of biodiesel produced.

4. Conclusions
The concentration of fatty acid methyl ester (FAME) using perforated helical type (as much as 86.26%) was higher than conventional helical type (as much as 82.79%) or increased by 4.06% (third scenario) and viscosity was decreased by 15.33% (third scenario) from conventional helix due to the presence of perforated helix. The addition of holes in conventional helix proven to increase the amount of FAME produced and improved the mixing and stirring processes that occur.

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