Numerical Simulation of Biodiesel Synthesis in T-Channel Microreactor

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Abstract. Biodiesel promising as an alternative to the diesel. The transesterification reaction process involved the reaction of triglyceride with alcohol in the presence of catalyst. In the research, the Computational Fluid Dynamic (CFD) method was used to simulate the transesterification reaction process. The inlet pressure range from 0.0001 Pa to 0.01 Pa, temperature of 25°C, 50°C, 75°C and the molar ratio at 6:1, 9:1 were used to investigate their effect of toward the biodiesel conversion. Finding shows that high conversion of biodiesel occurred at low inlet pressure of 0.001 Pa with temperature of 50°C and the ethanol to oil molar ratio at 9:1.

1. Introduction

The increasing of industrialization in the world is affected by the demand for the petroleum. According to the International Energy Agency, the estimation done with 53% of increasing the global energy consumption was foreseen by 2030. Although there are huge quantities of petroleum found under the Earth's surface, but it took millions of years to form, which means the oil supplies will run out. The depletion of fossil fuels promoted to find the alternative fuel which is biodiesel. Biodiesel can be a part of the sustainable energy in near future as other renewable resources such as sunflower oil and Jatropha curcas oil [1]. In the research, sunflower oil is chosen to synthesis of biodiesel due to the low content of free fatty acid (FFA). Even though sunflower oil is an edible oil and Jatropha curcas oil is non-edible oil, but the content of FFA of Jatropha curcas oil is higher than sunflower oil, which is can occur soap formation. The soap formation can lead to the decreasing of biodiesel conversion. This is the main reason why sunflower oil is chosen to simulate the biodiesel conversion in the research.

The majority of the biodiesel operated in the batch or continuous reactor that known as conventional technology. Considering the current drawbacks of conventional biodiesel production technology, new technology was proposed for better advancement process. The process intensification technology is one of the alternatives that use in order to overcome the problem that use conventional technology [2]. Process intensification is emerging equipment and operational method that promise spectacular improvement in process plant, reduce the size and also boost the production efficiency. Process intensification also provides more benefits to the future of chemical engineering.
Microreactor technology is one of the elements that involved in the process intensification technology. Microreactor can be defined as the chemical reactor of extremely small dimension used to allow mixing and reaction occur. By using microreactor, excellent mass and heat transfer performance can be achieved due to the high interfacial area [3]. Therefore, microreactor can enhanced mixing compared to the reactor in the production of biodiesel. Even though the microreactor having a small dimension, which means the fluid in laminar flow, but it can constant the product output quality better than the conventional technology used.

2. Numerical Simulation
The construction of T-channel microreactor geometry model was developed by using AutoCAD software and import to the COMSOL Multiphysics software. The two inlet and one outlet were set as the boundary conditions. The dimension as shown in the figure 1 below. The unit dimension of the geometry used was millimetre (mm).

For the meshing, the two-dimensional model used the physic-controlled meshing instead of user-controlled meshing. The element size of physics-controlled meshing was included normal, fine, finer, extra fine and extremely fine size. The smallest size used, the highest accurate of result obtained [4]. For the quality measure of element size, it was depending on the minimum element quality. There are no absolute numbers to present for what the quality should be due to the different requirement on the quality needed. In general, the minimum element quality of below than 0.01 are considered as very poor quality. The reaction engineering, transport of diluted species and laminar flow were selected for the physics interface to simulate the synthesis of biodiesel. The transesterification reaction equation as shown in the equation 1.

\[ \text{TG} + 3\text{A} \rightleftharpoons \text{GL} + 3\text{E} \]  
where TG is the triglyceride also known as the sunflower oil, A is the ethanol, GL is the glycerol and E is referred to the biodiesel. The transesterification reaction is reversible process which means the excess alcohol used to shift the equilibrium towards the product [5]-[7]. In the research, the different of inlet pressure range from 0.0001 Pa to 0.01 Pa was used to simulate the effect of temperature and alcohol to oil molar ratio towards the biodiesel synthesis in T-channel microreactor. The oil conversion was used to examine the reaction of biodiesel production in the T-channel microreactor by using equation 2.
Oil conversion (%) = \left( \frac{C_o - C_f}{C_o} \right) \times 100 \quad (2)

where \( C_o \) indicates the initial concentration of sunflower oil and \( C_f \) is the final concentration.

3. Result and Discussions

3.1 Concentration Profile

Figure 2 shows the concentration profile for the T-channel (T) microreactor at the operating condition of temperature and ethanol to oil molar ratio were 50°C and 9:1 respectively. The concentration profile represents the concentration of biodiesel obtained. The outlet red colour for T-channel (T) microreactor at 0.0001 Pa was the darkest, which means resulted the maximum biodiesel conversion. According to the colour shows at the T-channel (T) microreactor, the biodiesel conversion at 0.001 Pa was higher than 0.006 Pa. This is because the increment of pressure, the decrement of biodiesel conversion due to the less contact time between the reactants.
3.2 Effect of temperature toward the biodiesel conversion

![Graph showing the effect of temperature on biodiesel conversion](image)

**Figure 3**: The effect of temperature toward the biodiesel conversion for T-channel (T) microreactor

Figure 3 indicates the effect of temperature toward the biodiesel conversion for T-channel (T) microreactor. From the result obtained, clearly shows that the conversion of biodiesel for T-channel (T) microreactor at 50°C was higher compared to the temperature of 25°C and 75°C. For the inlet pressure at 0.0001 Pa, the highest biodiesel conversion was at temperature of 50°C and followed by 75°C and 25°C. In fact, when the temperature increase, the biodiesel conversion was decrease. But, in this case, the conversion of biodiesel at the temperature of 50°C was higher than 75°C. This is because the temperature at 75°C is beyond the normal boiling point of ethanol. The ethanol boils rapidly at 75°C and lead to the formation of large number of bubbles that can inhibit the mass transfer and decrease the conversion of biodiesel. This is can be proved by looking at the biodiesel conversion for T-channel (T) microreactor at 75°C was drastically decrease from the inlet pressure at 0.0001 Pa to 0.01 Pa, even at high temperature.

3.3 The effect of ethanol to oil molar ratio toward the biodiesel conversion

![Graph showing the effect of molar ratio on biodiesel conversion](image)

**Figure 4**: The effect of ethanol to oil molar ratio toward the biodiesel conversion for T-channel (T) microreactor
Figure 4 indicates the effect of ethanol to oil molar ratio toward the biodiesel conversion for T-channel (T) microreactor. The overall trend shows that when the value of molar ratio used was increases, the biodiesel conversion also increases. For the inlet pressure at 0.0001 Pa, the higher biodiesel conversion goes to the molar ratio of 9:1 while the lower biodiesel conversion goes to the value molar ratio at 6:1. This is because to shift the transesterification reaction process in forward direction, it is necessary to use either an excess amount of alcohol or to remove one of the products from the reaction mixture. The biodiesel conversion of T-channel (T) microreactor was rapidly decrease from 0.001 Pa to 0.01 Pa for the both molar ratio of 6:1 and 9:1 at 50°C. The trend clearly shows that the biodiesel conversion was rapidly decrease when the inlet pressure was increase.

4. Conclusions

In the research, the sunflower oil, ethanol and 0.75wt% of NaOH were used to simulate the biodiesel production. The CFD model for T-channel microreactor was constructed to investigate the effect of temperature and alcohol to oil molar ratio towards the biodiesel conversion. The physics interface that were selected including the reaction engineering, transport of diluted species and laminar flow. The inlet pressure ranges from 0.0001 Pa to 0.01 Pa, temperature of 25°C, 50°C and 75°C and the molar ratio at 6:1, 9:1 were simulated to investigate their effect toward the biodiesel conversion. The finding shows that the biodiesel can be produced by using T-channel (T) microreactor at all inlet pressure, temperature and molar ratio simulated. High biodiesel conversion occurred at 50°C and molar ratio of 9:1 with lowest inlet pressure of 0.001 Pa. Whereas the result at temperature of 75°C shows low biodiesel yield as the temperature was beyond the normal boiling point of ethanol.

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