CFD simulation of fatty acid methyl ester production in bubble column reactor

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Abstract. Non-catalytic transesterification is one of the method that was used to produce the fatty acid methyl ester (FAME) by blowing superheated methanol bubbles continuously into the vegetable oil without using any catalyst. This research aimed to simulate the production of FAME from palm oil in a bubble column reactor. Computational Fluid Dynamic (CFD) simulation was used to predict the distribution of fatty acid methyl ester and other product in the reactor. The fluid flow and component of concentration along the reaction time was investigated and the effects of reaction temperature (523 K and 563 K) on the non-catalytic transesterification process has been examined. The study was carried out using ANSYS CFX 17.1. The finding from the study shows that increasing the temperature leads to higher amount of fatty acid methyl ester can be produced in shorter time. On the other hand, concentration of the component such as triglyceride (TG), glycerol (GL) and fatty acid methyl ester (FAME) can be known when reaching the optimum condition.

1.0 Introduction

Biodiesel is an alternative diesel fuel that is currently being used as blended fuel for transportation. The most common method to produce biodiesel are through a process known as transesterification of vegetable oils or animal fats and an alcohol in presence of catalyst or without catalyst [1]. Replacing fossil fuels with biodiesel is mostly due to the environmental policies to reduce carbon dioxide emission which are known as the causes of global warming and greenhouse effect [2].

Bubble column reactor is a cylindrical vessel which equipped with a gas distributor at the bottom [3]. The gas bubbles will diffuse into the surrounding liquid and react with the dissolved reactants. The bubble column reactor is developed to produce fatty acid methyl ester (FAME) by blowing bubbles of superheated methanol vapor continuously into vegetable oil without using any catalyst [4]. There are two mode of operation that valid for bubble column which are semi batch mode and continuous mode. For continuous operation the gas and the suspension flow concurrently upward into the column and the suspension that leaves the column will be recycled to feed tank. For semi batch mode of operation, the suspension is in stationary condition which means that it is zero liquid throughputs and the gas is bubbling upward into the column [5]. Characteristics of fluid dynamics in the bubble column reactors has significant effects on the operation and performance of bubble columns. Besides that, the flow regimes in bubble columns is classified and maintained according to the superficial gas velocity employed in the column. Type of flow regimes in bubble column are homogeneous (bubbly flow) regime, heterogeneous (churn-turbulent) regime and slug flow regime [5]. Figure 1 shows the flow diagram of a reactor using non-catalytic transesterification [4].
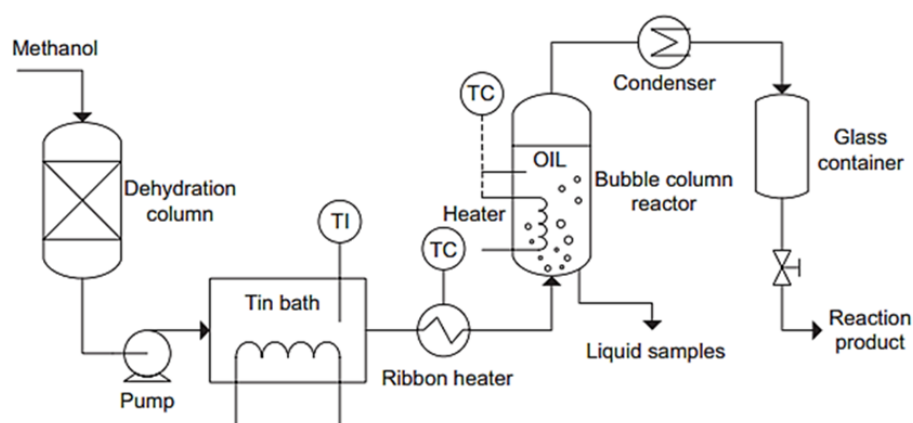
Figure 1. Schematic flow diagram of a reactor using non-catalytic transesterification experiment [4].

Computational fluid dynamic (CFD) model of a reactor developed in ANSYS software can be used to understand the physical and chemical process for the study. Development of CFD model allows different reactor designs (diameter and length) and operating conditions (flow rate) to be easily tested [6]. The ANSYS CFD software give valuable insight into a product's performance where it is delivered very well validated results to a model performance. Besides that, it is also capable of showing geometry for the computational domain and the various boundary conditions incorporated with the actual experiment setup. A study by Nikou and Ehsani (2008) shows the Computational Fluid Dynamics (CFD) model to describe the liquid to liquid flow phenomena observe in a reaction medium. The study has predicted the velocity distribution, pressure, concentration and temperature profiles in CFD model [7]. Therefore, this paper aim to predict the component concentrations in the bubble column reactor for biodiesel production and investigate the fluid flow inside the bubble column reactor during the reaction happens.

2.0 Methodology
Computational Fluid Dynamic (CFD) simulation by using CFX code which is consists in ANSYS 17.1 Workbench was used to investigate the fluid flow inside the bubble column reactor. For modeling the bubble column geometry, SolidWorks 2016 software was used. The diameter for bubble column reactor are referred from study conducted by previous researcher [4]. Material for bubble column reactor was selected to be stainless steel (316SS). The isometric view of bubble column reactor is shown in Figure 2.

The pressure in the bubble column was fixed 0.1MPa with temperature varied at 523 K and 563 K. For transient state solution, appropriate time step up was included to investigate the components concentration and fluid flow during the reaction time. On top of that, the meshing process was used to maintain a good quality of the cell. Then, the meshing model are runs in the solver process at reaction time for 1000 s. The boundary condition was used to determine the fluid flow directly toward the domain. The boundary condition are inlet, outlet and wall. The data setup for inlet was shown in Table 1.

Figure 2. The bubble column reactor

Table 1. Data setup for the inlet condition.

Parameter	Value
Velocity	2 m/s
Component concentration	Triglyceride = 0.59 x 10^3 mol/m^3 Methyl Ester = 12.3 x 10^3 mol/m^3

For this simulation, the outlet pressure was set to standard operating pressure at 101325 Pa. Then, along the wall was set to no slip boundary condition. For the material properties, the domain type are fluid domain which is contains methanol and palm oil (triglyceride, diglyceride and monoglyceride) in fluid database. Table 2 shows the properties for each fluid domains that are used in the simulation.

Table 2. Data for material properties.

Fluid Domain	Material properties
Methanol	Density = 791.8 kg/m^3 Viscosity = 0.59 mPa.s
Palm oil	Density = 870.2 kg/m^3 Viscosity = 16.93 mPa.s

3.0 Results

3.1 Fluid flow inside the bubble column reactor

The bubble column reactor was modelled for fluid flow at high gas velocities. The cross flow velocity within the bubble column were remained stable and did not change by time. In this condition, the bubble column reactor was analyzed at a steady state for different reaction temperature under atmospheric pressure. Figure 4 and 5 show the resulted velocity contour at the temperature of 523 K and 563 K for the bubble column reaction in XY Plane.

By increasing the temperature, it has affected the flow characteristic in the bubble column reactor. Red color in the Figure 3 shows the methanol in gas phase was started by blowing the bubbles of superheated methanol vapor at static pressure (0.1 MPa). The highest velocity was located at the inlet and become lowest when across the bubble column reactor. Then, blue color at Figure 3 represent the palm oil in the bubble column reactor at zero velocity. The effect of temperature was observed when the velocity magnitude increase to 563 K. It is found that by increasing the temperature, the velocity magnitude will increase.
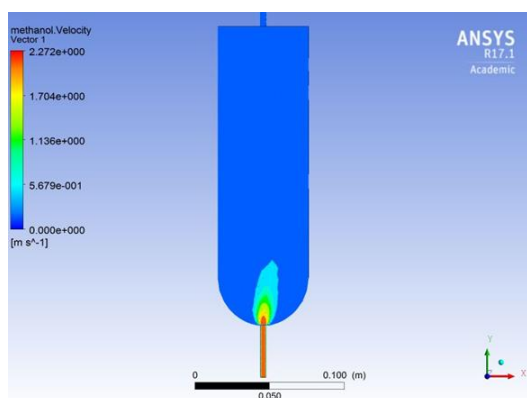
Figure 3. Contour of velocity in the bubble column reactor at steady state at 523 K
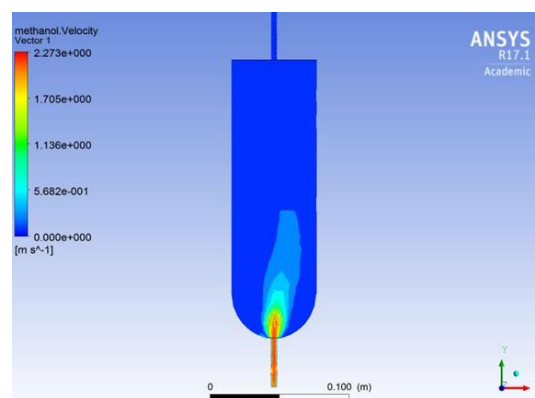

Figure 4. Contour of velocity in the bubble column reactor at steady state at 563 K

3.2 Contour for Component of concentration
The study deals with the component of the concentration from palm oil by using non-catalytic transesterification. Besides that, the result of the reaction in the component of the concentration should happen through of the bubble column reactor. Figure 5 and 6 shows the non-catalytic transesterification reaction for palm oil during the reaction.

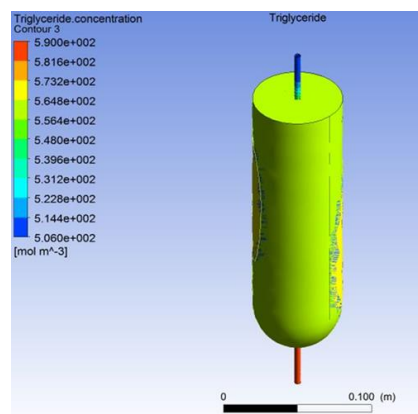**Figure 5.** Concentration contour for triglyceride at 523 K

Figure 6. Concentration contour of triglyceride at 563 K

Based on Figure 5 and 6 the changes in color were found because of the movement of materials depends on their viscosity, and there was more residence time for TG than other materials [8]. The difference in temperature increased the rate of chemical reaction [4]. Moreover, the raising in temperature can also increase the concentration of reactant in reactant gas. Methyl ester concentration from the simulation in bubble column reactor are shown in Figure 7 and 8.
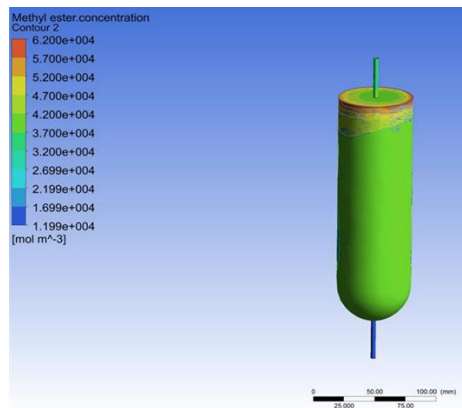
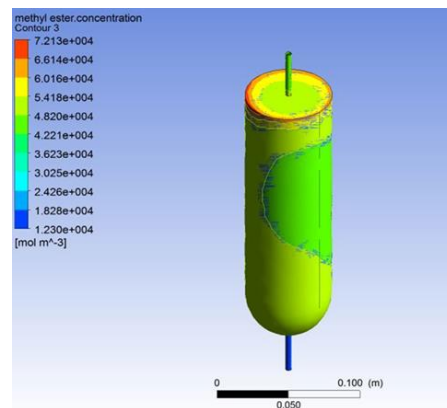**Figure 7.** Concentration contour of methyl ester at 523 K

Figure 8. Concentration contour of methyl ester at 563 K

The production of methyl ester was started earlier because of the first and second reaction in transesterification. Concentration of methyl ester are higher than triglyceride and glycerol. It is because methyl ester (ME) was produced by the three reactions in transesterification [4]. The blue contour at the bottom of reactor shows the initial reaction to produce ME.
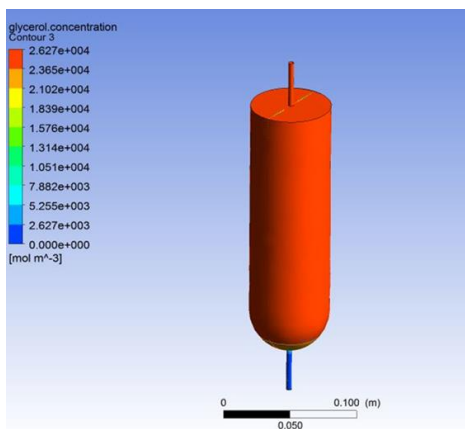

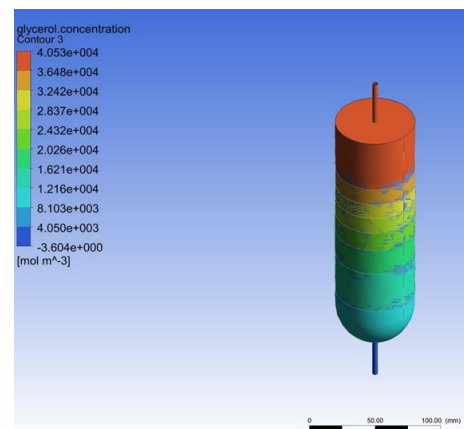**Figure 9.** Concentration contour of glycerol at 523 K

Figure 10. Concentration contour of glycerol at 563 K

Figure 10 shows the contour for concentration of glycerol at 563 K has changed color within the production process. The differences between patterns is depending on the increasing rate of their concentration which is much faster in methyl ester compared to glycerol because glycerol was produced only by the last reaction. On top of that, it was calculated by the interphase mass transfer process and the mixing which is caused by the bubbles. Otherwise, the effect of kinetic were depends on the reaction temperature so the two different temperature was selected to get two different reaction rates. All in all, when the temperature rise, it will make the reactant of particles move more quickly and more energy provided.

3.3 Graph for Component of concentration
The simulation result was compared with the finding of research conducted by Jeolianingsih et. al [4].
The trend indicates the reducing of the triglyceride concentration in experimental and simulation by
Computational Fluid Dynamics. Based on Figure 11, the experimental graph has slightly decreased
after 800s compared to the CFD graph that remained unchanged at 800s.
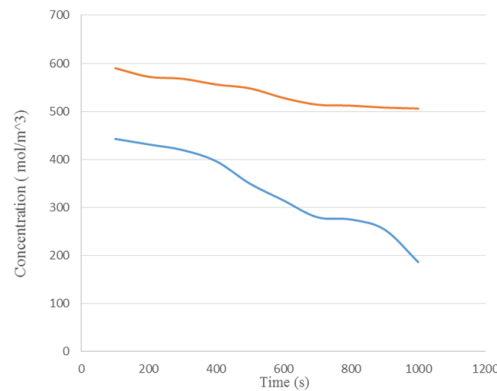

Figure 11. Concentration of triglyceride in bubble
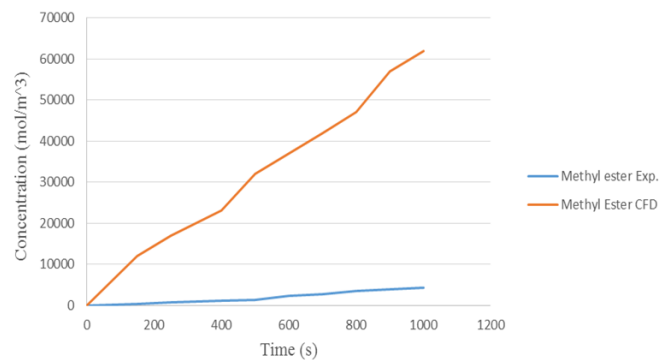column reactor at 563 K

Figure 12. Concentration of methyl ester in bubble
column reactor at 563 K

Figure 12 shows the concentration of methyl ester by simulation and experiment. In the initial
reaction, the production of methyl ester was rapid by simulation and experimental. Based on
Joelianingsih et. al [4], the increase in methyl ester will lead to increase in glycerol concentration at it
was liberated from triglyceride molecules. Thus, the conversion of the reaction of methyl ester
increased with reaction time and reaction temperature. The simulation result shows that the methyl
ester is produced at every 100 s but for the experiment, it started to changes at the 400s. This is due to
the velocity magnitude between the experiment and simulation. The velocity will lead to the
increasing in the concentration as well as will effect the component concentrations.
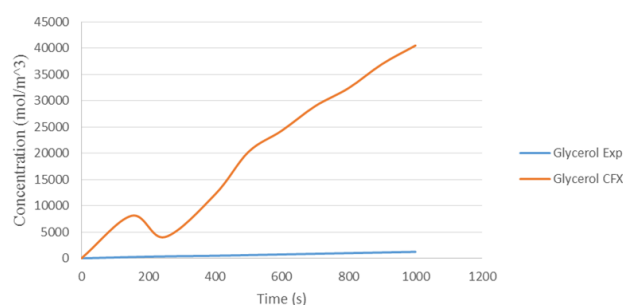
Figure 13. Concentration of glycerol in bubble
column reactor at 563 K

Figure 13 shows that the concentration for glycerol was rapidly increased in the simulation and maintained the same level at the experiment. The value for concentration in the experiment shows a slow changes at 500 s. Based on Jeolianingsih et al. [4], vapor pressure for glycerol was higher than triglyceride at the same reaction temperature thus the volatility of glycerol was higher than triglyceride [4].

4.0 Conclusion
The non-catalytic transesterification process shows that the production of biodiesel can be accomplished by using methanol at high pressure and temperature in BCR. By analyzing the component such as triglyceride (TG), diglyceride (DG) and fatty acid methyl ester (FAME) in BCR, the concentration can be shown along the process of producing biodiesel. Further study can be conducted to include the effects of molar ratio of oil to alcohol in simulation of biodiesel production in BCR.

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