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11-12 December, 2010 Inamori Foundation Memorial Building Center for Southeast Asian Studies, Kyoto University

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DETERMINATION ON CFD MODELING FOR BUBBLE COLUMN REACTOR TO IMPROVE BIODIESEL FUEL PRODUCTION

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ABSTRACT

Superheated methanol vapor bubble method has been developed to produce biodiesel fuel (fatty acids methyl esters; FAME) without using any catalysts at atmospheric pressure. This noncatalytic trans-esterification has an advantage over other trans-esterification methods at cost for production of biodiesel fuel. However, reaction rate is still lower than that of conventional alkaline catalytic method. Contact surface between the methanol bubble and the oil acts as the limiting factor for enhancing the reaction rate. Therefore, this study will be devoted to the analysis of the bubble size distribution during the process in the reactor using the Computational Fluid Dynamics (CFD) method. The aim of this report was to obtain optimum modeling of CFD to describe the bubble distribution in superheated methanol vapor bubble column reactor. Two dimensional (2D) and three dimensional (3D) models were used in this CFD simulation. Two types of wall function model were also accounted to characterize the high velocity and coalescence or breakup of bubble in the liquid. The relationship of intake gas velocity/coalescence and gas holdup/contact surface area was studied not only by computationally, but also by experimentally. As the results, the gas holdup and contact surface area in bubble column reactor became larger significantly when intake gas velocity was increased. 3Dturbulent and non-equilibrium wall function model showed best results in CFD simulation. This CFD modeling will be useful to improve the design the bubble column reactor.

Keywords: biodiesel fuel, bubble column reactor, computational fluid dynamics (CFD), modeling.

INTRODUCTION

Bubble column reactor is widely used in bio- and petro-chemical industries, such as biodiesel production. They are known as excellent reactors for processes which require large interfacial area for gas-liquid mass transfer and efficient mixing for reacting species. Recently, industrial biodiesel is produced by catalytic method by using alkaline and acid catalyst, where methanol and oil are reacted under vigorous mixing, at atmosphere pressure and temperature of 60°C by existing of catalyst to produce biodiesel and glycerol as by-product. Glycerol is the important substance for cosmetic, medical and chemical industry. However the method has a problem, in processing of biodiesel, it is needed the de-acidification and refining of catalyst from by-product of biodiesel. In order to solve the problem, we had developed one of non-catalytic biodiesel fuel processing technology which is called superheated methanol vapor bubble column where superheated methanol vapor flowed in the oil in the bubble column reactor under atmosphere pressure and temperature of 250°C-300°C to produce biodiesel and glycerol. Biodiesel and glycerol can be separated in easy way (by using distillation and sedimentation process). The operation and processing cost hence is reduced by using non catalytic method. However, the reaction rate of biodiesel production still lower than that of catalyst method.

Previous studies [1] declared that bubble size distribution of superheated methanol vapor was very importance parameter to enlarge the surface contact area between methanol and oil, hereinafter to enhance the reaction rate of biodiesel production. Bubble size distribution was a hydrodynamics phenomenon, where two phases of gas and liquid were being in the bubble column reactor. The use of CFD method should be able to explain the bubble behavior, by providing a complete description of the local hydrodynamics if an adequate model is used [2]. Determination of model in the CFD is important to obtain the best result as well as the method of CFD verification. Producing of biodiesel

by using superheated methanol vapor in the bubble column reactor take place under atmosphere pressure and need high temperature ($250^{\circ}C - 300^{\circ}C$), hence reactor was made of stainless-steel and covered by insulation. In deal with verification of CFD modeling, it was not able to show the bubble distribution. Therefore the transparent bubble column reactor was used to display the bubble size distribution by utilizing of nitrogen gas and water as simplification.

The objectives of the research are to verify the CFD modeling and to determine the CFD modeling appropriately for describing the bubble distribution behavior in the bubble column reactor by implementing the comparison between the CFD modeling and result experiment.

CFD MODELING (ASSUMPTION AND BOUNDARY CONDITION)

The model of bubble column reactor was implemented into CFD code ANSYS FLUENT (version 6.3.26 and version 12.1.21) and the geometry or mesh of reactor modeling was constructed using GAMBIT 2.4.6. The multiphases model (two phases) was used in the bubble column CFD modeling. Two and three dimensional simulations have been carried out for the bubble column configuration. Volume of Fluid (VOF) model was used to represent the interaction of two phases (gas and liquid). No mass and no heat transfer are considered. Both of laminar and turbulent models (standard k- ϵ approach) were used in the simulations. Due to the narrow reactor where gas flows close to the wall of reactor, two models of wall function were used in the CFD modeling; standard wall function and non-equilibrium wall function. In all simulations, unsteady numerical solution was obtained.

The boundary condition included inlet and outlet applied the inlet velocity and pressure velocity, respectively. Due to the open system simulation, the initial pressure in the gas space above the liquid column was equal to the atmospheric pressure (101.325 kPa). The continuum boundary condition consists of liquid at height of 12.43 cm (from the bottom of reactor) and vapor (at the upper part of reactor). The value of backflow of liquid volume fraction was one which indicated that gas phase only could pass through the outlet. The value of liquid volume fraction at the inlet boundary condition was zero which indicated that gas phase only could entrance through the inlet.

EXPERIMENTAL SET UP

The transparent bubble column reactor model was made at same scale with bench scale super heated methanol bubble reactor by acrylic. The diameter of reactor vessel was 55 mm and 220 mm height with a gas inlet at the bottom. The reactor was filled with distilled water (H =124.3 mm, at 25 °C). Nitrogen gas was flowed from central nozzle (diameter of 4.8 mm) at the bottom of reactor vessel. The inlet velocity (flow rate) of nitrogen gas varies at 0.276 m/s (0.3 L/min), 0.921 m/s (1 L/min), 1.842 m/s (2 L/min), 2.763 m/s (3 L/min) and 5.32 m/s (5.770 L/min) allowing the laminar and turbulent regimes to be investigated. The bubble size distributions were obtained using digital camera.

RESULTS AND DISCUSSION

CFD Verification

Two dimensional (2D) simulations had been conducted to elaborate the significance of 3D work. The gas bubble behavior in the reactor vessel was obtained by digital camera with high-speed Sutter (Figure 2, 3).

Figure 2 shows the laminar 2D and 3D CFD modeling compare by experiment results at gas inlet velocity of 0.276 m/s. The 2D computation gave the quite different of bubble distribution in comparison with 3D computation and result experiment. Moreover, 2D computational could not to carry out at velocity more than 1.842 m/s, due to the liquid spill from the reactor for superficial gas velocity over than 1.842 m/s. This phenomenon indicated that no reasonable to used 2D computation for the model of bubble column reactor.





3D CFD modeling gave the same trends of bubble distribution as the experiment result especially for low intake gas flow. For high intake gas flow, the simulation was the same as the experiment result for bubble size and the pattern of bubble distribution, but not for shape of bubble. The simulation revealed the oval bubble shape, whereas the experiment generated the round bubble shape.

The difference was expected due to the influence of turbulence model still not enough to revealed the real condition. Because of the high Reynolds number for the airflow gas(> 1.842 m/s), where the big bubble rise and gave a tendency to collision to result coalescence or break-up, it will be better to use non-equilibrium function model which strong recommended to the impingement where the mean flow and turbulence are subjected to severe pressure gradients and change rapidly. Using the non-equilibrium wall function–3D model to account the collision to result coalescence or break up for high Reynolds number in the simulation gave better results than standard wall function model, that expressed by the shape of round bubble obtained in Figure 3(b).





The effect of gas velocity inlet to gas holdup and surface contact area were studied in the present work. Gas holdup is the basic parameter indicating the hydro-dynamical characteristics of bubble columns. It affects directly the geometric sizes of bubble columns, and the gas-liquid interfacial area thus affects the mass-transfer rates of bubble columns. So it is one of the necessary and important

parameters for the design of bubble columns [3]. As a result, both of contact surface area and gas holdup increase with increasing gas velocity. This result matches with that of the other researchers [4],[5], [6], [7].

CONCLUSIONS

Determination of the best CFD modeling to describe the bubble distribution in the reactor was investigated. The 3D CFD modeling, turbulent flow and non-equilibrium wall function gave the best similarity with experimental result. The effects of inlet gas velocities to the gas holdup and contact surface area were accounted. The increasing of inlet gas velocities caused increasing of the gas holdup and contact surface area significantly.

Furthermore, the best CFD modeling determined in present work will be used to simulate the reactor using methanol vapor and triglyceride as liquid to obtain the best design of reactor nozzle for producing the highest reaction rate.

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