INVESTIGATION ON TRANSESTERIFICATION OF BIODIESEL BY MOLECULAR MODELLING

INTRODUCTION

In the recent years, the use of fossil fuel is the direct effect to the economical crisis. To solve this problem is searching for an application of material or substance in domestic to decrease the fuel demand from import. The use of diesel oil is in the high rate compared with the other fuels. Hence, the diesel fuel demand is the key factor on Thai economic growth. From this reason, the government supports the diesel price to slowdown the economy. Beside that the government has a strategy to support a research for the new compensation energy such as gasohol and biodiesel.

Vegetable oils have the potential to substitute for petroleum fuel in the near future. Vegetable oils fuels are not competitive with petroleum fuel now because vegetable oils are more expensive than petroleum fuels. However, because of the increasing of petroleum fuel prices and the uncertainties problem availability, there is an interest in using vegetable oils in diesel engine. Vegetable oils have good heating power and provide exhaust gas with almost no sulfur and aromatic polycyclic compounds. But there have been many problems associated with using it directly in diesel engine (especially in direct injection engine). These include; coking and trumpet formation on the injectors to such an extent that fuel atomization does not occur properly or even prevented as a result of plugged orifices, carbon deposits, oil ring sticking, thickening or gelling of the lubricating oil as a result of contamination by vegetable oils, lubricating problems (Meher, 2004), and was limited due to its high viscosity (near 10 times of the gas oil) (Carmen et al., 2005). The main process that has been investigated in attempts to overcome those drawbacks and improve the properties of vegetable oils is called “Transesterification” or “Alcoholysis” (Srivastava et al., 2000).

Biodiesel, defined as the mono-alkyl esters of fatty acid that is derived from vegetable oils or animal fats, has demonstrated a number of appreciating characteristic include reducing of exhaust emission. It is a substitute for diesel fuel was demonstrated by the inventor of the diesel engine, Rudolph Diesel, around the year 1900, when vegetable oil was proposed as fuel for engines. It is derived from a renewable, domestic resource, thereby relieving reliance on petroleum fuel imports. It is biodegradable and non-toxic. Compared to petroleum-based diesel, biodiesel has a more favorable combustion emission profile, such as low emissions of carbon monoxide, particulate matter and unburned hydrocarbons. Carbon dioxide produced by combustion of biodiesel can be recycled by photosynthesis, thereby minimizing the impact of biodiesel combustion on the greenhouse effect (Körbitz, 1999; Agarwal and Das, 2001). In brief, these merits of biodiesel make it a good alternative to petroleum based fuel and have led to its use in many countries, especially in environmentally sensitive areas (Zhang, 2003).

As a consequence of biodiesel properties and advantages, there is considerable interesting to support and promote the use of biodiesel fuel. Computational techniques are being used in this study to help researchers for better understanding of Biodiesel Production with the new approaches and without spending unnecessary materials and expense in exercising the experiment.

Objective

To study and simulate structural and energetic properties of triolein and transesterification mechanism by molecular modelling.

Scope of work

1. Study a transesterification of biodiesel using heterogeneous catalyst.
2. Find an exact structure or possible structure of triolein with a lowest molecular energy to complete the transesterification mechanism

3. Simulate all proposed transesterification mechanism to find the possible mechanism of the reaction.

4. Using GaussViewW and GUASSIAN 03W to do a simulation.

Expected results

1. Use simulations to investigate possibility the biodiesel reaction.

2. Improve the transesterification of biodiesel production reaction using heterogeneous catalyst.