CONCLUSIONS

This thesis focuses on the simulation of critical substance; triolein, in transesterification of biodiesel production to find the best conformation of triolein molecule with the lowest molecular energy and to propose the possible transesterification mechanism pathway. The transesterification mechanism study starts with the determination of geometrical parameters of triolein molecule. Three methods AM1, PM3 and *ab initio* HF give a good agreement. As a result, the model of triolein molecule can be used in the simulation of transesterification mechanism. These simulations part are performed by GAUSSIAN 03W and GaussViewW.

The active site distances were found from the simulation. The first active sites is a site between carbon atom in carbonyl group of glyceride (C=O) and oxygen atom of methoxide. The second active site is a site between oxygen atom that is next to the carbon atom in carbonyl group of glyceride (C=O) and hydrogen atom of methanol. These two active sites were based on transesterification mechanism in Fig. 3. The distance between glyceride and methoxide varies in a range of 1.4300 to 1.6000 angstrom (Å). The distance between product of the first reaction (intermediate1 or product in step 1) and methanol varies from 0.9 to 1.2 Å. Next, the all of reactions in transesterification mechanism were simulated based on semiempirical PM3 to find the minimum reaction distance. Therefore, the minimum distance of the reaction between carbon atom in carbonyl group of glyceride (C=O) and oxygen atom of methoxide is 1.5165 Å. The minimum distance of the reaction between product of the first reaction (intermediate1 or product in step 1) and methanol is 1.1000 Å. An angle between carbonyl group and methoxide (O=C-O) is 90 degree. The *ab initio* Hartree-Fock was simulated all of reactions again for more accuracy. And two input files are proposed in each of glyceride mechanism because of step2 and step3 are combined together as the result from this simulation

Totally, the six types of transesterification mechanism or thirty six reactions were studied based on an *ab initio* Hartree-Fock method with 3-21G and 6-31G basis

set. From the simulations found that the types of the reactions were divided into six types;

1. The first type is irreversible reaction that the output molecule structure is product.
2. The second type is irreversible reaction that the output molecule structures are reactants instead of product.
3. The third type is irreversible reaction that the output molecule structure is similar to the product but the active site bond wasn't shown.
4. The forth type is reversible reaction that the output molecule structures are reactants instead of product.
5. The fifth type is reversible reaction that in the final the reaction doesn't give product.
6. The sixth type is reversible reaction that the output molecule structure is similar to the product but the active site bond wasn't shown.

The energy of the reactant in each step of transesterification mechanism is higher than the energy of the product. The energy in each type of the reaction in transesterification mechanism is similar to the other. The possible transesterification mechanisms are found in all types of transesterification mechanisms.