Pojanee Krongsinsuk 2009: Pathway Analysis of Transesterification Reaction of Palm oil using Base Catalyst. Master of Engineering (Chemical Engineering), Major Field: Chemical Engineering, Department of Chemical Engineering. Thesis Advisor:
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This research aims to clarify the pathways of the transesterification of triglycerides (TG) and methanol using potassium hydroxide as a catalyst. Experiments were performed in a batch system, 400 rpm, 20 ^{o}C and the molar ratio of oil to methanol at 1:6. To clarify the pathway of the tranesterification of TG, detection of positional isomers of *sn*-DG and *sn*-MG is needed. The equipment for identifying TG, DG, MG, ME and GL in the reaction mixture of transesterification reaction are HPLC, MS and NMR.

In this experiment, the samples were taken at 20 min and kept for the isolation of compounds. After that it was confirmed by MS analysis to consider the molecular species. The isolated compound was matched with the molecular species of TG, DG, MG and ME. From the mass spectrum analysis showed that the alkyl chain of these compounds predominated the palmitic, oleic and linoleic fatty acid. For ^{1}H NMR method, the isolated compounds were determined with respect to a resonance signal of proton and expected to distinguish the positional isomers of *sn*-DG and *sn*-MG. The result showed that, there were 2 positional isomers on *sn*-DG (*sn*-1,2-DG and *sn*-1,3-DG). For MG, the mixture of *sn*-1-MG and *sn*-2-MG was found. All these compounds were used as the standard for HPLC analysis to identify the chromatogram. The experimental result demonstrated that, the amounts of *sn*-1,3-DG was higher than *sn*-1,2-DG during in the reaction. To support the experimental result, the computational technique was used to determine the minimum molecular energy of *sn*-1,2-DG and *sn*-1,3-DG, it showed that the structure of *sn*-1,3-DG was more stable than *sn*-1,2-DG. It could be explained by the selectivity in the reaction that involved the formation of mainly *sn*-1,3-DG over *sn*-1,2-DG. All of these analyses showed that the transesterification reaction occured easily at *sn*-2-position for both TG and DG. Our results suggested that the most possible pathway was the attack of methoxide ion to the carbonyl group of TG which occurred easily at *sn*-2-position to form *sn*-1,3-DG. After that, methoxide ion attacked at *sn*-1(3)-position of *sn*-1,3-DG to form *sn*-1-MG. In the last step, *sn*-1-MG reacted with methoxide ion to get glycerol and biodiesel.

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