

## CHAPTER VII

### CONCLUSIONS AND RECOMMENDATIONS

#### 7.1 Conclusions

In this work, it has demonstrated that the deoxygenation of methyl octanoate can effectively take place over the H-ZSM5 catalyst. The reaction initially occurs through the condensation and hydrolysis, leading to the formation of 8-pentadecanone and octanoic acid as primary products. Consequently, the variety of hydrocarbons is formed via cracking reaction of the pentadecanone and octanoic acid. The comparative study conducted with n-octane as a reactant suggests that aromatics are produced through a series of reactions; cracking, oligomerization, and cyclization. However, the aromatization of the methyl octanoate over the H-ZSM5 can occur more effectively than that of n-octane. Moreover, it was observed that the direct dehydrocyclization of the methylester can take place over the H-ZSM5, but it is not evident for the reaction of n-octane.

As compared to the H-ZSM5 catalyst, it was found that the Zn/H-ZSM5 insignificantly improves the aromatic yield. By contrast, a significant improvement of the aromatic yield is attained from the reaction of n-octane on the Zn/H-ZSM5. This is because the zinc cation enhances the conversion of olefin compounds (aromatic precursors) into the aromatics. Furthermore, the presence of Zn species does not promote any alternative reaction routes. Similar to the H-ZSM5 catalyst, one of the dominant aromatization paths involved in the reaction of methyloctanoate is the direct ring closure forming o-xylene. This path most probably occurs via activation of the H atom bonded to the C in the  $\alpha$  position relative to the carbonyl group. That is, the oxygenated compounds maybe aromatized before deoxygenation.

When the reaction of the 10 wt% of methyl octanoate methanol was investigated over the CsNaX catalysts, it exhibited that the decarbonylation / deacetalation activity of methyl octanoate can occur at high rates and better stability due to the presence of fragments of methanol on the surface, compared with the reaction when nonane was co-fed. The methanol fragments are in the form of

formate-like species that also inhibits the formation of the high molecular weight molecules. Heptenes and hexenes are produced as major products from the decarbonylation of the methyl octanoate, proceeding through an octanoate-like species as intermediate from the decomposition of the methylester. The hydrogenation and hydration also take place over the CsNaX catalysts using the surface hydrogen from the methanol decomposition. When the washing was applied to the CsNaX catalyst, a significant loss of the cesium species was found, leading to the decreases in the basic strength and the generation of acid sites. The excess cesium species does not provide the additional decarbonylation activity. As a result, hexenes were obtained in higher amount than heptenes from the washed CsNaX catalysts. It is believed that hexenes arises from the decomposition of the cyclic-like intermediate on the acid sites. If the cesium is absent from the catalyst (NaX zeolite), the basicity is much lower and the weak acid sites become dominant, resulting in the production of undesired products, such as multi-substituted aromatics, and the decrease in decarbonylation/ deacetalation. Although the MgO catalyst is known as a basic solid catalyst, its low activity indicates that the highly polar environmental characteristic of the zeolite is necessary for the reaction.

## 7.2 Recommendations

Although the H-ZSM5 catalyst showed an excellent activity in the deoxygenation of the methylester, the yield to light hydrocarbons gas is still high due to its high acidity. It is defied to reduce the cracking activity and improve the aromatization activity. The addition of other metals might be helpful for this issue. Furthermore, the utilization of the Cs exchanged zeolite X catalyst seems to be another effective application for the conversion of the methylester to hydrocarbons. Therefore, it is interesting to practically apply the reaction in the refining of biodiesel with low hydrogen consumption.