# CHAPTER VI

# CONCLUSIONS AND RECOMMENDATION

In this research, the catalytic activity of TS-1 and TS-1 modified with second metals, V, Al, Co and Fe are determined. The performance of the catalysts is evaluated and the reaction mechanisms of product formation during the hydroxylation of toluene and ethyl benzene with hydrogen peroxide are proposed. The experiment, result and discussion are summarized in the first part of chapter and another part is recommendation. At the end of this research the following conclusions and suggestion for future work are drawn.

## 6.1 Conclusions

TS-1 and M-TS-1 are synthesized by hydrothermal and second metals are added by incorporation in the step of synthesis. All catalysts have the MFI structure and the presence of $Ti^{4+}$ in framework following normal characteristic of TS-1. The acid site of TS-1 and M-TS-1 can be organized into three groups i.e. weak acid site, strength acid site and strong acid site.

The catalytic activity of toluene hydroxylation is observed at 70°C and 95°C. The reaction at 70 °C gives products as p-cresol, o-cresol for all catalysts. Al-TS-1 and Fe-TS-1 also have benzaldehyde. The total conversion of toluene to products follows order: Fe-TS-1 (10.01%) > Al-TS-1 (5.39%) > TS-1 (1.09%) > Co-TS-1 (0.85%) > V-TS-1 (0.34%) and the selectivity of product observed follows sequence : TS-1 > Co-TS-1 > V-TS-1 > Al-TS-1 > Fe-TS-1. The formation of products have affected from (i) the structure of toluene molecule which prefer substation at ortho position, (ii) the kinetic diameter and shape of products which affect molecular diffuse out of catalyst pore and (iii) the position at which toluene molecule attaches on active site of catalyst. Furthermore, second metals affect capability of organic reactant adsorption. The amount of toluene adsorbed on catalysts follows order: Fe-TS-1 > Al-TS-1 > TS-1 > Co-TS-1 > V-TS-1. Therefore, Fe-TS-1 and Al-TS-1 have much reactant on catalyst surfaces which leads to high conversion.

The hydroxylations of toluene at 95 °C over TS-1 and M-TS-1 (except Fe-TS-1) have o-cresol and benzaldehyde as the main products. p-cresol is found only with Co-TS-1 and V-TS-1 but with lesser amount than at 70 °C.

The predominant products obtained from ethyl benzene hydroxylation at 70 °C and 95 °C are acetophenone and 1-phenethyl alcohol. In addition, Fe-TS-1 also produces phenethyl alcohol and benzalacetaldehyde.

The product formation mechanisms of toluene and ethyl benzene hydroxylations are explained by the electrophilic aromatic substitution mechanism and hydrogen peroxide free radical mechanism. The cresol products are obtained from benzene ring oxidation while the side chain oxidation products (benzaldehyde and all products of ethyl benzene) can be formed via two mechanisms. The first one is the same mechanism as products from ring oxidation and the other one is hydrogen peroxide free radical mechanism.

## 6.2 Recommendations

From the previous conclusions, the following recommendations for future studies are proposed.

(1.) The catalysts synthesis has several parameters which influencing performance and catalyst properties, therefore, these affecting parameters should be identified and investigated.

(2.) Other acid solution for the pretreatment of TS-1 catalysts should be tried.

(3.) Since the toluene hydroxylation can yield high benzaldehyde, an important intermediate of perfume synthesis, this system may be adapted to be a choice for benzaldehyde production

(4.) In the experiments, the fresh catalysts are only used in the reaction. Further study on catalyst stability and regeneration is still needed.