CHAPTER V
CONCLUSIONS AND RECOMMENDATIONS

5.1 Conclusions

In this study, the liquid phase adsorption of three refractory sulfur compounds (3-methylthiophene, benzothiophene and dibenzothiophene) in simulated fuels (isooctane and decane) was investigated by using ion-exchanged zeolite. Metal Ni^{2+} and Cu^{2+} metal ions were selected to exchange with NaY zeolite in this study. The amount of metal loading was varied by changing the solution : adsorbent ratio (S:A) which was found to increase with increasing the S:A ratio in the ion-exchange process. From ion exchange isotherms, it was found that Na^{+} in NaY zeolite can be replaced by Ni^{2+} and Cu^{2+} for 67.19% and 57.59% of the total cations, respectively. In the adsorption of the three sulfur compounds in simulated fuels, all the isotherms were found to be fitted with Langmuir isotherm. Thus, the Langmuir parameters (q_{max} and k) could be determined. From the results of adsorption of three sulfur compounds, NiY zeolite was not affected from the amount of Ni^{2+} loading and they were almost the same with NaY zeolite before ion exchange. It can be concluded that loading Ni^{2+} on Y zeolite does not improve the sulfur adsorption capacities of the NaY zeolite. In contrast to NiY, CuY zeolite showed significantly higher adsorption capacities and adsorption affinity towards sulfur compounds than NaY zeolite. Also, the ability in adsorbing the sulfur compounds improved with increasing the amount of Cu^{2+} loading.

In prediction of the interaction parameters in combining rules of Kwak and Mansoori, the CO_2 + 2,2,2-Trifluoroethyl Methacrylate system (Kwon *et al.*, 2007) was selected to verify the Peng-Robinson model. In their experiment, the interaction parameters of kij and lij were -0.0258 and -0.0234, respectively. By using FORTRAN to evaluate the interaction parameters in this experiment, they were -0.0215 and -0.0244 for k_{ij} and l_{ij}, respectively. So, this program can be used to predict the interaction parameters in other systems.

5.2 Recommendations

5.2.1 Sulfur Adsorption

The effect of pore size of zeolite should be studied by synthesizing the new zeolite that has the appropriate pore size to fit with the structure of sulfur compounds. From the increasing in amount of sulfur adsorption when increasing the amount of Cu^{2+} loading, the effect of temperature during ion exchange should be studied to increase the amount of Cu^{2+} loading which may lead to higher the adsorption capacities.

5.2.2 Adsorption in the Presence of Supercritical Fluid

In this part, the modeling of the equilibrium adsorption should be considered to reduce the time and cost in doing an experiment. From these equations,

$$\left(\frac{\partial \ln K_2}{\partial T}\right)_p = \frac{(h_2^{IG} - \bar{h}_2^m) + \Delta H_2^{ads}}{RT^2} + \alpha^m \tag{5.1}$$

$$\left(\frac{\partial \ln K_2}{\partial P}\right)_T = \frac{\bar{\upsilon}_2^m}{RT} - \kappa^m \tag{5.2}$$

there are two alternative ways in determining the adsorption equilibrium constants (K_2).

1. If adsorption equilibrium constant is known at various temperatures, equation (5.1) was applied in order to determine ΔH_2^{ads}. Because the heat of adsorption is independent of chemical structure of the solute but it depends on the type of sorbent, this heat of adsorption can be applied for other solutes with the same sorbent. Thus, K-T diagram can be predicted for other solutes if the adsorption equilibrium constant at one temperature is known. Also, the adsorption equilibrium constant at various pressure can be predicted if equation (5.2) is applied. Next, the Langmuir isotherm is generated.

2. If there are experimental data at various temperature and pressure such as the equilibrium constant at 313 K, 104.4 bar and 318.1 K, 119.8 bar, equation (5.2) should then be used to translate data at 318.1 K, 119.8 bar to 318 K, 104.4 bar and equation (5.1) can be applied which is followed the case 1. Consequently, the

adsorption equilibrium constant can be predicted at various temperature and pressure. Therefore, the Langmuir isotherm is generated at various temperature and pressure.