CHAPTER VI
CONCLUSIONS AND RECOMMENDATIONS

6.1 Conclusions

In this thesis, we studied the continuous liquid adsorption of three refractory sulfur compounds (3-methylthiophene, benzothiophene, and dibenzothiophene) in simulated transportation fuels (gasoline and diesel) on NaX zeolite. The effects of initial sulfur concentration and type of sulfur compounds on the adsorption breakthrough curve were examined. The desorption of sulfur compounds was also studied by heating the column at 400°C. Furthermore, the mathematical model of the sulfur adsorption on NaX zeolite was developed to predict the breakthrough curves. The experimental results indicated that at higher initial feed concentration, the slope of the breakthrough curve is steeper and the breakthrough time is shorter due to a large driving force accelerating the adsorption rate. Whereas, the breakthroughs of the three types of sulfur compounds are found to arrange in the order of BT>3-MT>DBT. The slowest breakthrough point of BT results from the preferential adsorption due to the presence of benzene ring in its structure which can interact with zeolite acidic surface via π-bonding. While the earliest breakthrough point of DBT is influenced by the steric hindrance effect on the adsorption of a relatively big molecule. For the desorption study, the desorption of spent NaX with adsorbed 3-MT and BT were successfully achieved while the recovered adsorption capacity of NaX that adsorbed with BT is a slightly lower than that adsorbed with 3-MT. It was also found that for 3-MT and BT, there was no difference in the recovered capacity of NaX between 1 hour and 3 hours heating. However, this technique appears not to be effective for the desorption of DBT. This is probably due to the strong interaction between two benzene rings in DBT's structure and acidic zeolite surface which make it difficult to desorb the adsorbed sulfur compound.

A mathematical model assuming biporous structure for NaX zeolite particle was developed to predict the breakthrough profiles under various conditions.

Through the use of the model, the dynamic adsorption of sulfur compounds could be explained by the combined effects of liquid film mass transfer, diffusion in the macro-pores and within the crystals of the zeolites pellet. The results show that the breakthrough curves generated from the model agree reasonably well with the experimental data. In addition, the adjustable parameter could be adjusted for higher initial sulfur concentration.

6.2 Recommendations

Upon the completion of this study, the adsorption of three major thiophenic compounds in transportation fuels using Na-based faujazite zeolite was established. It is interesting to further study towards the modification of faujasite zeolite by loading various metal ions on zeolites. Effect of the amount of exchanged metal in zeolite on sulfur compounds adsorption should be also investigated in details. Heavy metals such as Zn, Ni, and Cu are potential candidates for the modification of the faujasite zeolite. Subsequently, comparison between Na-based faujasite zeolite and zeolite loaded with other metal ions for their surface adsorption capability can be done.

For the model development, the model sensitivity analysis should be done to assess other parameters that may have significant effect on the characteristic breakthrough curve or time. In addition, other experimental conditions should be studied to evaluate the precision in breakthrough curve predicting.