ADSORPTION EQUILIBRIUM OF MIXED ORGANIC SOLVENT TO FAU TYPE HIGH SILICA ZEOLITE

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Introduction

When the solvent collection device like the PSA method is designed, it is very important to know the adsorption equilibrium relations between adsorbent and adsorbates, and movement and adsorption speed of adsorbates in absorbent intergranular. The molecular simulation method is an effective method to the examination of the adsorption mechanism to the zeolite at a molecular level. Especially, the GCMC simulation is used to predict the adsorption equilibrium. The GCMC simulation is a technique for changing a lot of atoms and the positions of the molecule one after another according to the stochastic process by random numbers that generate it, and calculating there by the balanced structure and amount of thermodynamics.
In this study, it made comparative study of the simulation that used Materials Studio with the gravimetric method adsorption experiment.

Experimental

Gravimetric Method

Gravimetric analysis was used to obtain the adsorption curves plotted for the ratio of volumes of solution ($qt/q\infty$) against time (t). Micropore diffusivity was obtained by analyzed adsorption curve. The amount adsorbed was measured corresponding to the pressure of the vapor in the tube. The pressure was measured by pressure sensor at higher pressure range (> 0.013 atm) and baratron at lower pressure range (<0.013 atm). A Time with increment value of adsorption was measured by chart recorder. In this way, the adsorption curves were obtained.

In this research, FAU type zeolite (SiO_2/Al_2O_3=460) was used as sorbate and ethanol and trichloroethylene were used as adsorbates. The adsorption equilibrium experiment used the gravimetric method. By using the zeolite of about 0.25g, adsorbates were poured from a high vacuum of pressure 10-6atm and measured the weight change in the absorbent with a differential transformer.

Simulation

Materials Studio

Simulation module in Materials Studio (Accelrys Inc.) was used throughout MC simulations. As for Materials Studio, the adsorption equilibrium can be reproduced in a short time, and two or more calculations are possible at the same time. The power place used cvff that corrected Universal. Ratio of the silica alumina (SiO_2/Al_2O_3) of the FAU type zeolite that is saved in the library of MS was adjusted to 460 and the absorbent was used. It calculated by the Sorption module, and the adsorption isotherm was obtained.

Result And Discussion

The adsorption isothermals that obtained from the gravimetric method experiment and GCMC simulation are shown in Fig.1 and Fig.2.
Result of simulation of two elements is shown in Fig.3. And adsorption equilibrium curve according to total concentration.

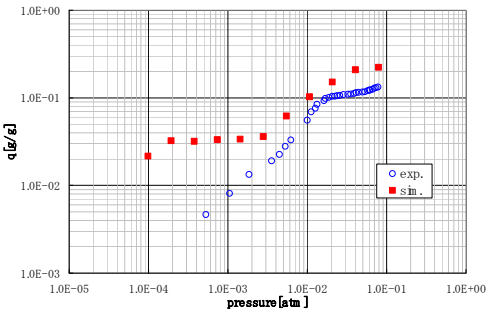

Fig.1 Comparison between experiment and simulation(adsorbate: ethanol)

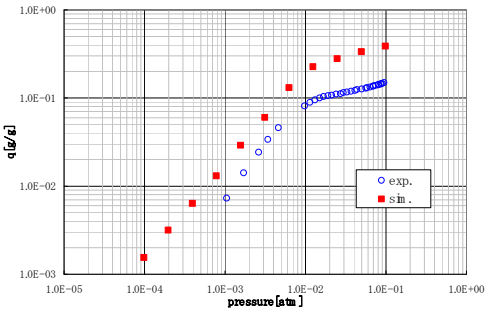

Fig.2 Comparison between experiment and simulation(adsorbate: trichloroethylene)

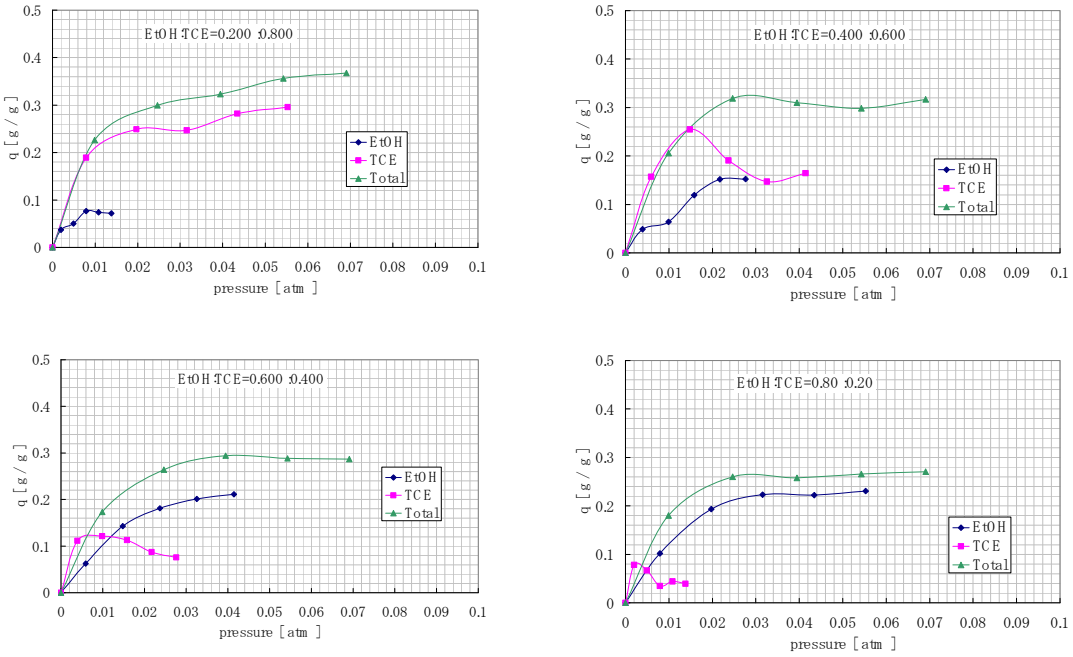

Fig.3 Result of simulation of two elements

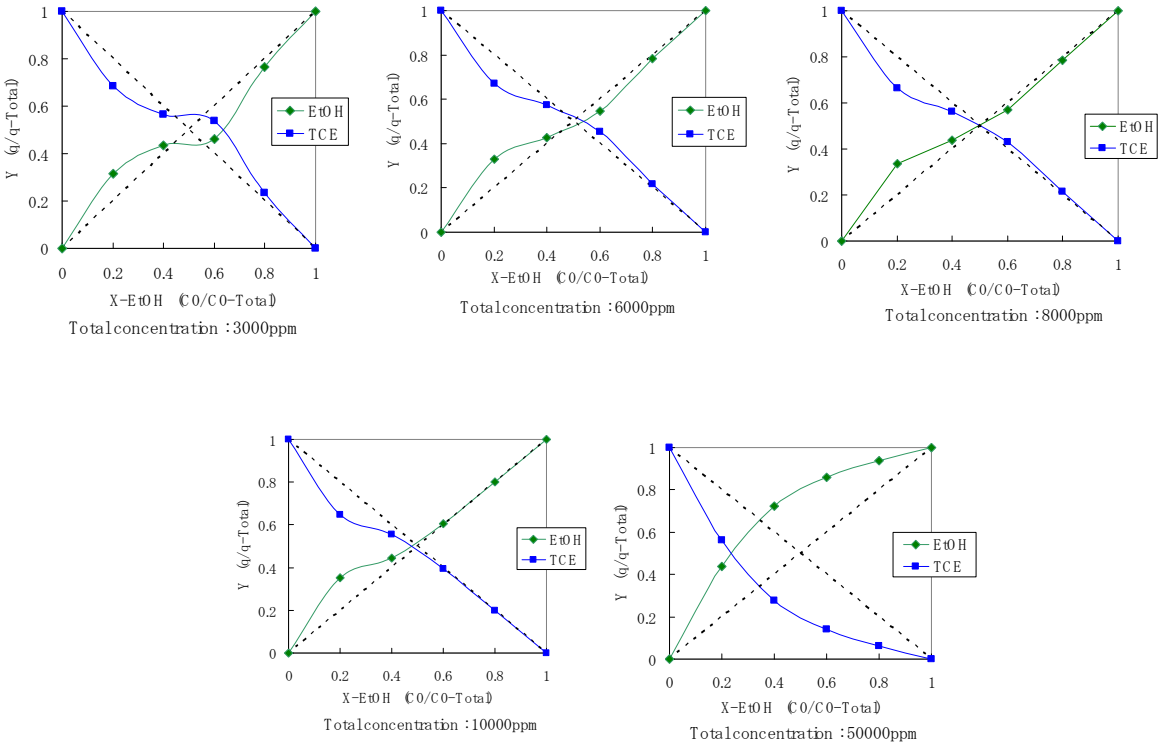

Fig.4 Adsorption equilibrium curve according to total concentration

Conclusions

The value of the amount of the equilibrium adsorption was able to be calculated as a tendency in MS(Fig.1, 2). In accuracy, the amount of adsorption of MS is greatly different compared with the weight method experiment. It will be necessary to improve the crystal structure and the calculation condition of MS in the future. Moreover, the value and the adsorption equilibrium curve of the adsorption equilibrium experiment of two elements of the amount of the equilibrium adsorption were able to be calculated as a tendency in MS(Fig.3, 4).

References

1. K. Chihara, M. Suzuki, K. Kawazoe, Adsorption rate on Molecular Sieving Carbon by Chromatography, AIChE, 24,237(1978)