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Adsorption of Organics on MSC5A in Supercritical CO_2, Chromatographic Measurements & Stop & Go Simulation

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1. Introduction

Chromatographic measurements were made for the adsorption of benzene, toluene and *m*-xylene on molecular sieving carbon (MSC) in supercritical fluid CO_2 mixed with organics. Supercritical chromatograph packed with MSC was used to detect pulse responses of organics. Adsorption equilibria and adsorption dynamics parameters for organics and CO_2 were obtained by moment analysis and stop & go simulation of the response peaks. The dependencies of adsorption equilibrium constants, K^*, and micro pore diffusivity, D, of benzene, toluene and *m*-xylene, on the amount adsorbed with each parameters of temperature or pressure were obtained. It was found that the values of K^* and D for an organic substance depended on the amount adsorbed of other organics strongly.

Stop & Go method was used as simulation method of perturbation chromatography for investigating adsorption equilibrium and rate. Numerical solution for multi component chromatogram in time domain could be obtained by appropriate model equations with experimental conditions. This simulated chromatogram can be compared with experimental chromatogram to determine the adsorption equilibrium and rate parameters.

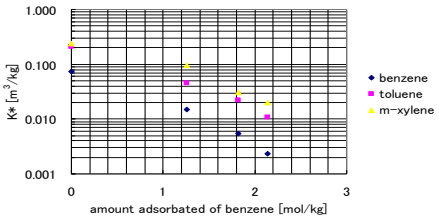

Figure.1 Dependencies of K* on the amount adsorbed of benzene

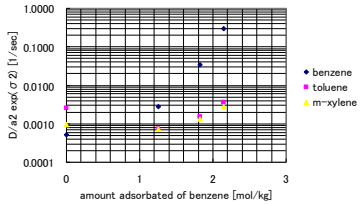

Figure.2 Dependencies of D/a2 exp(σ2) on the amount adsorbed of benzene

2. Results and Discussions

The apparent adsorption equilibrium constant, K* and time constant of micropore diffusivity, D/a2 exp(σ2) obtained from first and second moment of response peak, as in Fig. 1 and 2.

Co-adsorption isotherm for CO_2 + benzene like Fig. 4 was determined by comparison like Fig. 3. Then, Co-adsorption isotherm for CO_2 + benzene + *m*-xylene was supposed to simulate like Fig. 5.

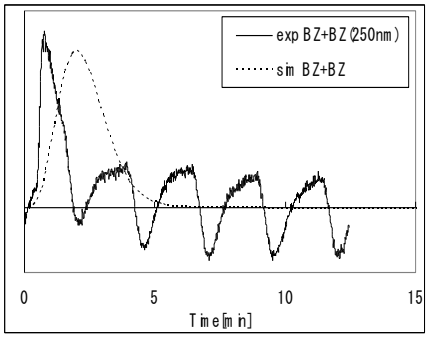

Figure 3, Comparison between experimental and simulated pulse response (carrier: CO_2 + benzene, pulse: benzene, 150 atm, 313 K, 0.03 ml/min benzene)

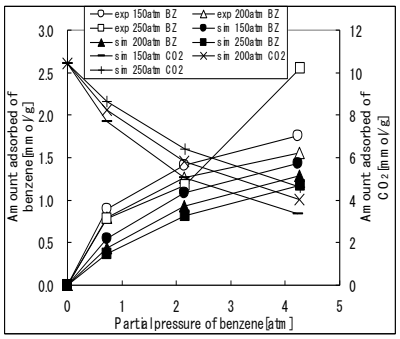

Figure 4, Comparison between experimental and simulated adsorption isotherm (carrier: CO_2 + benzene, pulse: benzene, 150 atm, 313 K, 0.03 ml/min benzene)

3. Conclusion

Adsorption equilibrium and adsorption dynamics on MSC were evaluated for each organics in supercritical CO2 fluid mixed with adsorbate by chromatographic measurement. The dependencies of adsorption equilibrium constants, K*, and micropore diffusivity, D, of benzene, toluene and m-xylene, on molarity of benzene, toluene or m-xylene with each parameters of temperature or pressure were obtained, respectively. It was found that the values of K* and D for an organic substance depended on the amount adsorbed of other organics strongly. In the stop & go simulation, the experimental amount adsorbed and adsorption rate could be almost simulated.

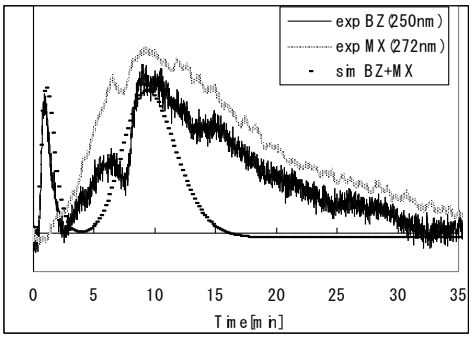

Figure 5, Comparison between experimental and simulated pulse response (carrier: CO_2 + benzene, pulse: *m*-xylene, 150 atm, 353 K, 0.03 ml/min benzene)

References [1] K. Chihara, K. Oomori, T. Oono and Y. Mochizuki, *Water Science and Technology 35, 7* (*1997*) *261–268*.

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