

diffusion-fundamentals

The Open-Access Journal for the Basic Principles of Diffusion Theory, Experiment and Application

Diffusion of BTX in MSC5A in Supercritical CO₂

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1. Introduction

Separation by adsorption in supercritical fluid might have some possibility. There, diffusion in micropore of adsorbent might be a controlling factor. In this study, chromatographic measurements were made for the adsorption of benzene, toluene and m-xylene on molecular sieving carbon (MSC) in supercritical fluid CO₂. Supercritical chromatograph packed with MSC was used to detect pulse responses of organics. Adsorption equilibria and adsorption dynamics for organics were obtained by moment analysis of the response peaks. Dependences of apparent adsorption equilibrium constants, K^* , and micropore diffusivity, D, on the amount adsorbed were examined.

2. Result and discussion

Figure 1 shows adsorption isotherm of benzene at 313 K. According to Fig.1, the amount adsorbed increased with increases of molarity of benzene, and reached to saturation. The amounts adsorbed became larger with decreases of column pressure. It was considered that the situation is competitive adsorption and amount adsorbed of benzene decreases as CO₂ adsorption increase with increases of column pressure.

Figure 2 shows dependency of adsorption equilibrium constants, K^* , for benzene, toluene, and m-xylene on amount adsorbed of benzene at 20 MPa. This is reasonably decreasing.

Fig.3 shows dependency of micropore diffusivity, $D/\bar{a}^2 \exp(\sigma^2)$, for benzene, toluene, and m-xylene on amount adsorbed of benzene at 20 MPa. The increase of $D/\bar{a}^2 \exp(\sigma^2)$ for benzene could be reasonably explained by chemical potential driving force. However, as for dependency of $D/\bar{a}^2 \exp(\sigma^2)$ of toluene and m-xylene on amount adsorbed of benzene, further discussion would be necessary.

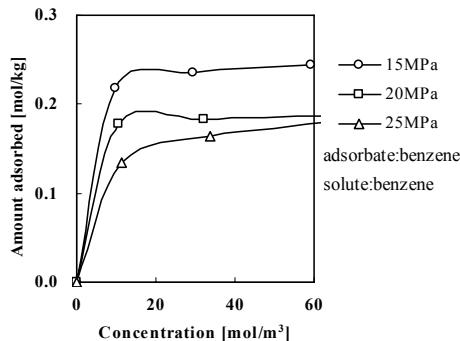


Figure 1. Adsorption isotherm : benzene at 313K

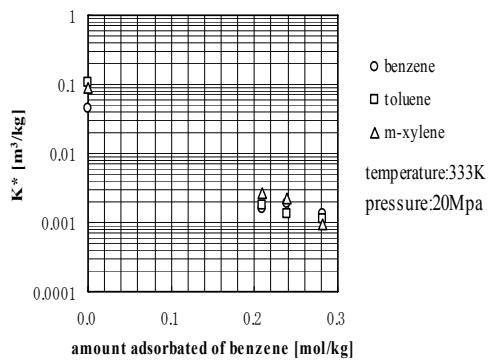


Figure 2. Dependencies of K^* on the amount adsorbed of benzene

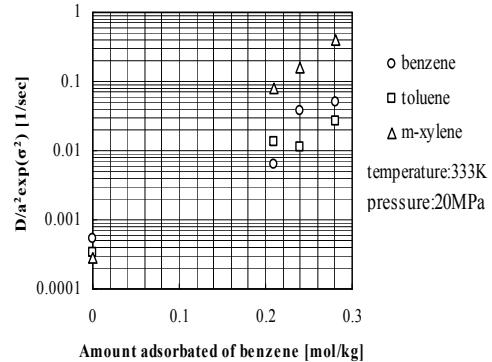


Figure 3. Dependencies of $D/a^2 \exp(\sigma^2)$ on the amount adsorbed of benzene

Figure 4 shows contribution of four mass transfer steps of benzene in pulse response (μ'_2). The effect of micropore diffusion is dominant in all the conditions examined.

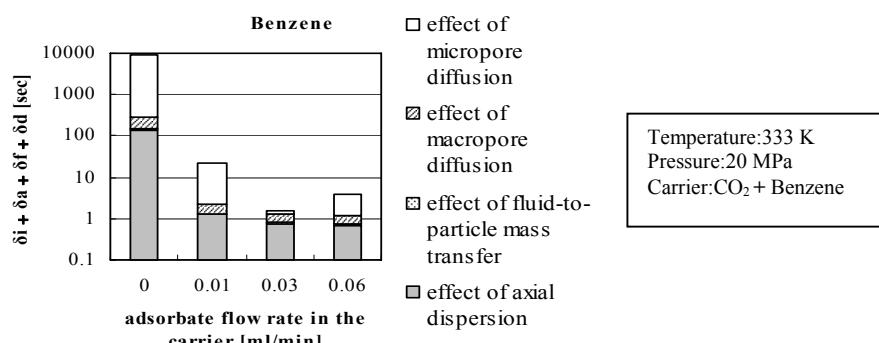


Figure 4 Contribution of four mass transfer steps

3. Conclusion

Adsorption equilibrium and adsorption dynamics on MSC were evaluated for each organics in supercritical CO_2 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.

References

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