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Diffusion Study of Multi-Component Gas Adsorption in MSC5A by Chromatographic Method

Kazuyuki Chihara, Hidenori Nakamura, Yosuke Kaneko

Department of Applied Chemistry, Meiji University, 1-1-1 Higashi-mita, Tama-ku,
Kawasaki, Kanagawa, 214-8571, Japan, E-mail:chihara@isc.meiji.ac.jp

1. Introduction

The combination of chromatographic method and moment analysis of the response peaks is one of the useful techniques to study adsorption equilibrium and adsorption rate [1]. Perturbation chromatography with the mixed multi component adsorbate gas carrier (two adsorbates) has been applied to several studies on adsorption [2][3]. In this work, perturbation chromatography with multi-component gas carrier (two adsorbates with inert gas) and non-equilibrium thermodynamics linear law was applied for discussion of the interference effect and the displacement effect (those are cross effects) on mass transfer in multi-component gas adsorption as previous study for different gas mixture (He, N_2, CH_4) [4]. Moment analysis method and stop & go simulation method were utilized to obtain each mass transfer parameter of adsorbate gases. Dependency of micropore diffusion on amount adsorbed and correlation of micropore diffusion with chemical potential driving force for microporous adsorbent were discussed. Also, cross effects were discussed. Ruthven already emphasized the dependency of micropore diffusivity on amount adsorbed in single component adsorption [5]. Tondeur et al gave general background on multi-component perturbation chromatography for the first moment only [6].

2. Experimental method

The apparatus was similar to a conventional gas chromatograph. Adsorbent particles were packed in a column. Carrier gas was a mixture of two or three components among He, CO_2, CH_4. Perturbation pulse was introduced into the carrier gas stream. Introduction of pulses was performed by 6-way valve. The pulse size was 1cc, which meant injection period was 1.4 sec. Then pulse response was detected by TCD cell. Output signal of TCD was transmitted to a personal computer through RS232C. This signal was also transmitted to the personal computer. Simulated chromatogram by a personal computer can be overlapped on experimental chromatogram shown in the monitor screen. Further, moment of pulse response, which is shown in the monitor screen, can be automatically calculated by the personal computer.

3. Result and Discussion

Fig.1 shows an example of comparison of experimental chromatogram with simulated chromatogram for MSC5A to obtain *Ksav* for LDF model. Experimental conditions were 313 K, column pressure 5 atm, flow rate 25 cm/sec and He+CH_4 mixed gas carrier with CH_4 pulse. Here CH_4 concentration in the carrier gas was changed 10, 30, 50, 70 and 90 %.

Fig.2 shows contribution of axial dispersion, external mass transfer, macropore diffusion and micropore diffusion in case of CH_4 for MSC5A at 323 K. This figure illustrated that mass transfer is controlled by micropore diffusion. Fig.3 shows the dependency of micropore diffusivity coefficient of CO_2 with amount adsorbed at 303, 313 and 323 K for MSC5A. Fig.4 shows the correlation of micropore diffusivity of CO_2 with chemical potential driving force at 303, 313 and 323 K for MSC5A. Proportional relation was obtained, which means that micropore diffusion is based on chemical potential driving force.

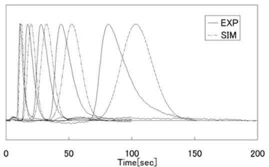

Fig. 1 Comparison of experimental peaks with simulation

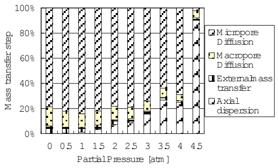

Fig.2 Mass transfer steps of CH_4 on to MSC5A

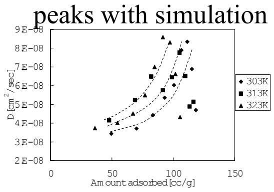

Fig. 3 Dependency of micropore diffusivity coefficient on the amount adsorbed

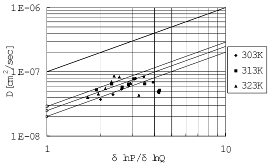

Fig.4 Correlation based on chemical potential driving force

4. Conclusion

This time, we cannot get good agreements between experimental chromatogram and simulated chromatogram, based on the modeling of Stop & Go method, in case of perturbation chromatography with mixed adsorbate gas carrier. And micropore diffusivities obtained were interpreted by chemical potential driving force consideration based on non-equilibrium thermodynamics law. Some possibility was shown for a cross-effect of micropore diffusion in multicomponent adsorption.

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