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Azeotropic Adsorption of Organic Solvent Vapor Mixture on High Silica Zeolite, Mass Transfer Dynamics

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Introduction

Discharge of organic substances into air has been strongly prohibited since some decades ago, to preserve comfortable natural environment. Though hydrocarbons, alcohols and chlorinated hydrocarbons had been used as the degreasing agent in industries, these solvents may also affect to our environment, and it is necessary to remove them from air as much as possible. This study was performed aiming at presenting useful data for the design of adsorption processes, especially the removal of the solvent vapors, as above, from air by adsorption. The solvents used were trichloroethylene (TCE) and ethanol (EtOH). Further, the experimental breakthrough curves of the EtOH-TCE system was simulated using the STOP&GO method[1], which accounted mass balance and mass transfer in divided cells of the adsorption column. γ /Ksav was the key parameter as for over all mass transfer, including the micro pore diffusion, when comparing the result of a simulation with an experiment result.

Experimental

Solvents used were ethanol (EtOH), trichloroethylene (TCE). Adsorbents were packed in a glass column of 0.10m length and 0.0156m i.d. Experimental conditions were as follows: linear flow rate; 0.2 m/s, influent concentration; in the range of 0.004~0.2 mol/m^3, and temperature; 298 K.

Breakthrough Curves with Simulation

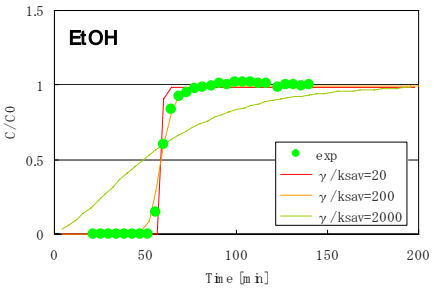
Since Langmuir equation was not able to be used for this binary systems, in which adsorption equilibrium data, two azeotropic points were observed, the following equation (1) was used. The equation of the azeotropic theory in a liquid-vapor azeotropic equilibrium was applied instead of Langmuir equation.

$$Y_i \gamma_i P_i = X_i P \qquad (1)$$

where Pi* is the vapor pressure and γi the activity coefficient of component i.

The activity coefficient was first calculated from experimental data. The relation between a gaseous phase molar fraction and the activity coefficient are plotted. γ vs. X equation was obtained by curve fitting of this plot. This equation was substituted into Eq.

(1) to get equation two correlations between a gaseous phase molar fraction and an adsorbed phase molar fraction. Stop & Go method for simulation of breakthrough curve with these correlations was applied to get Figure 1. Breakthrough curves were almost simulated in all cases. Over all mass transfer coefficient based on amount adsorbed $\gamma/K_s a_v$ was obtained as 200 [sec], because of the best fit to the experimental breakthrough curves.



Discussion

Obtained $\gamma/K_s a_v$ includes the effects of axial dispersion, film mass transfer, macro-pore diffusion & micro-pore diffusion as follows,

$$\frac{1}{K_S a_v} = \frac{\beta}{K_F a_v} = \frac{\beta}{k_F a_v} + \frac{1}{k_S a_v} + \frac{d_p \beta}{Pe \cdot u}$$

$$\frac{1}{(k_S a_v)_{overall}} = \frac{1}{(k_S a_v)_a} + \frac{1}{(k_S a_v)_i}$$

$$(k_S a_v)_a = 15 D_{pa} (1-\varepsilon)/\beta R^2$$

$$(k_S a_v)_i = 15 D_{si} / a^2$$

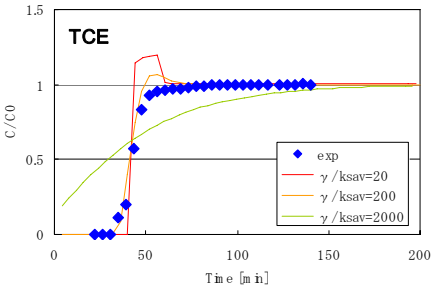


Fig.1 Comparison of experimental breakthrough curve with simulation.

By estimation of all other effects, micro pore diffusivity D_{si}/a^2 was obtained from $\gamma/K_s a_v$ as 5.8×10^{-6} [1/sec](EtOH), 8.7×10^{-7} [1/sec](TCE), Here, almost all the mass transfer resistance was in micro pore diffusion.

Conclusion

Adsorption of some organic solvent vapors onto HSZ was studied. Binary adsorption equilibrium except azeotropic mixture-HSZ systems could be correlated by Markham-Benton equation for the whole concentration range. However, two azeotropic points appeared in the adsorption equilibrium for EtOH-TCE-Y-type system. For this binary systems, adsorption equilibrium data could be expressed by proposed equation, similar to liquid-vapor azeotropic equilibrium equation. Breakthrough curve could be simulated using the Stop & Go method in the whole range for this azeotropic mixture systems to get micro pore diffusivites.

Reference

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