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

Competitive Sorption of Toluene and Acetone on H-ZSM5 Zeolite: Comparison between Molecular Simulation Calculation and Experimental Results

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1. Introduction

We here present a study of sorption of toluene/acetone mixtures on the popular, commercial zeolite H-ZSM5. Experimental results are compared with theoretical data obtained by molecular simulation which has allowed determination of both sorption isotherms and the equilibrium uptake of a gaseous mixture at selected pressure and temperature. Both are of some importance given the wide industrial use of toluene and acetone. Toluene occurs naturally in crude oil and is also produced in the process of making gasoline and other fuels from crude oil. It is used in making paints, paint thinners, adhesives, and rubber and in some printing and leather tanning processes. Acetone, of course, is a flammable manufactured chemical that is used to make plastic, fibres, drugs, and other chemicals. It is also used to dissolve other substances.

A successful understanding of the separation mechanism in this type of materials requires a good description of both the diffusional and the equilibrium properties of gaseous mixtures in zeolite pores.

Such factors can be now calculated by molecular simulations, pioneered as long ago as 1938 by Barrer [1] and developed recently with more sophisticated algorithms [2,3]. The Grand Canonical Monte Carlo (GCMC) method [4] have been used successfully in recent years to study adsorption of gases in microporous materials such as zeolites.

2. Results

As reported elsewhere [5], the number of molecules sorbed depends mainly on their volume and charge distribution. Calculations show that acetone sorbs more highly than does toluene throughout the temperature range selected in both selected zeolites and at the same pressures. A constant sorption is observed for both compounds up to a certain temperature, above which the sorption decreases dramatically in particular when the more acidic zeolite (at lower pressure) is used. Even more interesting is the result obtained simulating the sorption of a toluene/acetone mixture, reported in Table 1. It can be observed that the competition favours acetone sorption and that at room temperature only acetone is adsorbed.

The results of experiments carried out in gas phase at 673 K, in saturated vapour environment at 298 K, and in batch at 273 K, were in good agreement with calculations. The kinetics of adsorption of the 1/1 (v/v) toluene/acetone mixture in batch is shown in Figure 1

Table 1. Sorption of toluene (1kPa)/acetone (1kPa) gaseous mixture on H-ZSM5/35

T/K	Acetone molecules/supercell	Toluene molecules/supercell
300	89	0.0
600	18	32

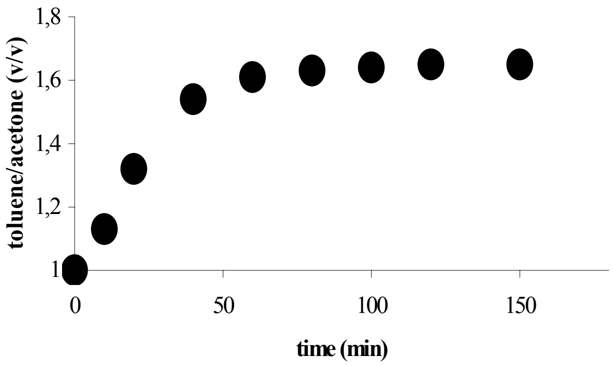

Fig. 1. Toluene/acetone ratio in the supernatant solution during the sorption of 25 μL on 5 mg of H-ZSM5/235.

3. Conclusions

Molecular simulation shows that there is a competition between acetone and toluene for sorption on H-ZSM5 zeolites. Independent of the pressure and the zeolite acidity, 89 molecules of acetone and 34 molecules of toluene are sorbed by a supercell of the zeolite, at least in the temperature range 300-450 K, when the calculations are done separately. However, when an equimolar gaseous mixture is sorbed, only acetone uptake occurs at room temperature. The same competition is also observed for liquid solutions, where the acetone sorption is favoured with respect to that of toluene. This result can open a new route for using zeolites as stationary phases in liquid chromatography. In the gaseous phase at room temperature, acetone and toluene vapours are sorbed in the same amount in the acid zeolites, while the absence of acidity favours the acetone uptake. The same results are obtained when the temperature is increased up to 500 K. At higher temperatures both compounds are sorbed.

References

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