The Competitive Diffusion of Gases in a Nanoporous Zeolite Using a Slice Selection Procedure

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The study of the co-diffusion of several gases through a microporous solid and of the resulting instantaneous distribution (out of equilibrium) of the adsorbed phases is particularly important in many fields, such as gas separation, heterogeneous catalysis, etc. Classical H NMR imaging is a good technique for visualizing these processes but, since the signal obtained is not specific for each gas, each experiment has to be performed several times under identical conditions, and each time with only one incompletely deuterated gas. In contrast, we have proposed a new NMR imaging technique (based on the so-called NMR slice selection procedure) which gives a signal characteristic of each adsorbed gas. It can therefore provide directly, at every moment and at every level of the crystallite bed, the distribution of several gases competing in diffusion and adsorption. Solutions to the direct and inverse problems are based on Heaviside's operational method and Laplace integral transformation. New procedures for identifying diffusion coefficients for co-diffusing components (benzene and hexane) in intra- and intercrystallite spaces were implemented, using high-speed gradient methods and mathematical diffusion models, as well as the NMR spectra of the adsorbed mass distribution of each component in the zeolite bed. These diffusion coefficients were obtained as a function of time for different positions along the bed. Benzene and hexane concentrations in the inter- and intracrystallite spaces were calculated for every position in the bed and for different adsorption times.