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Exploring diffusion and reaction in nanoporous catalysts by IR micro-imaging

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Though PFG NMR has been successfully employed for the in-situ measurement of the diffusivities of the various components during chemical reactions [1] it fails to provide any information about the location of these components. Recent progress in the development of in-situ techniques for the characterization of solid catalysts [2] has overcome this limitation and provided us, with IR micro-imaging [3], with a technique offering best prospects for the recording of transient concentration profiles of the involved components during chemical reactions. The present contribution introduces into these options.

As an alternative to diffusion-reaction studies in zeolites with two-dimensional channel networks, we have cared for the option of similar investigations with three-dimensional pore networks. For this type of measurement, the catalyst is applied in the shape of small platelets, with the two large faces covered with a suitable layer which is impenetrable for the guest molecules but IR transparent at the relevant frequency. Hence, by observing perpendicular to the plane of the platelets, any diffusion in observation direction is excluded and IR micro-imaging directly yields the concentration profiles, simultaneously for each individual component!

First results of this type of measurement in a nanoporous glass [4] are shown in Figure 1. In order to show the potentials of our model-system in combination with IR micro-imaging we performed a so called counter-diffusion experiment. The sample is thereby pre-loaded with benzene and then suddenly exposed to a cyclohexane atmosphere. In Figure 1 the benzene concentration in the sample is clearly seen to decrease (a, b) while, at the same time, the concentration of cyclohexane is increasing (c, d). Concentration profiles can be recorded because the coating of the glass plates ensures that the molecules can only enter from the open side on the right and not through the surfaces on top or bottom.

We are presently performing experiments for demonstrating these potentials by recording the spatial distribution of the components involved in simple model reactions like the reduction of benzene to cyclohexane.

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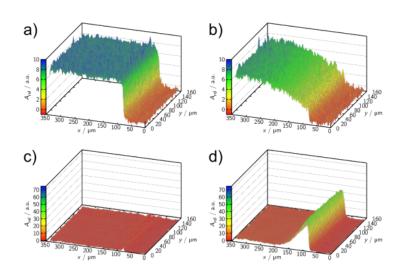


Figure 1: Concentration of benzene (a, b) and cyclohexane (c, d) before (a, c) and 20 s after (b, d) the replacement of benzene by cyclohexane in a counter-diffusion experiment