THE EFFECTS OF EXTERNAL SURFACE BARRIERS ON DIFFUSION AND REACTION IN ZEOLITE CATALYSTS

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Zeolites are attractive heterogeneous catalysts due to their crystalline structure, high surface area and thermal stability. However, conventional zeolites display diffusion limitations in many relevant catalytic processes. The slow diffusion rate through the extended network of micropores leads to low catalyst utilization and can, furthermore, lead to reduced selectivity and catalyst lifetime [1]. One nature-inspired approach to decrease diffusion limitations is to use hierarchically structured porous materials with an optimized network of broad and narrow pores. Observations in nature can help to provide a mechanistic basis to design the optimal pore network, since the architecture of nature is dominated by hierarchical structures. Hierarchical transport networks are indeed common in many natural systems, such as the respiratory and circulatory systems, as well as in leaves. At large length scales transport is dominated by convective flow, while at smaller length scales transport is dominated by diffusion [2]. Thus, the incorporation of hierarchical porosity can enhance the diffusion and reduce or even eliminate diffusion limitations in zeolite catalysts [3]. In addition to enhanced catalyst utilization, increasing the external surface area and maximizing the rate of intracrystalline diffusion could also lead to improved catalyst life times.

Nevertheless, recent experimental and computational work suggests that external surface barriers in zeolite-based, hierarchical catalysts might play a significant role in affecting overall transport and reaction rates in such catalysts [4]. Rao et al. [5] demonstrated the existence and impact of surface barriers on the alkylation of benzene with ethylene by comparing reactor simulations with experimental results.

In recent work in our group, ZSM-5 zeolites with similar bulk properties were prepared with different external surface properties, using different synthesis methods and conditions. The synthesized materials were studied extensively using different characterization techniques to determine their chemical, structural and textural properties. This set of catalysts was then used for appropriate catalytic experiments to investigate the impact of surface barriers on the catalytic properties of zeolites. This knowledge will be important to understand how surface barriers can be either avoided or exploited.

References

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