Combinatorial neutron imaging for in-situ alkane adsorption analysis over C_1-C_4 coupling catalysts

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Hydrocarbons are essential commodity chemicals used in various applications and crucial for our society. However, their dependence on fossil sources puts pressure on the environment. Hence, the production of these molecules from renewable sources is crucial for the advancement of a sustainable society. Currently, the most promising routes rely on the activation and subsequent oligomerization of small molecules (C_1-C_4) into longer chain hydrocarbons over heterogeneous catalysts. Nevertheless, these systems suffer from poor selectivity towards a single target product,[1] as well as rapid deactivation.[2] These transformations are largely governed by the ability of the reagents and products to diffuse though the catalyst pore network. Therefore, a complete understanding of the sorption kinetics is beneficial for the establishment of descriptors that aid the design of catalytic materials with optimized properties. Such investigations are traditionally performed by infrared radiation (IR) in combination with Raman spectroscopy or by simple gravimetric methods.[3] While these methods provide valuable information on the properties of a system, the in-situ optical visualization of the material changes during the adsorption/desorption process remains challenging due to interferences with the source light. In addition, the design of suitable cells is required for the application of these techniques under realistic temperatures and pressures. Herein, the uptake and desorption kinetics of *n*-hexane as probe molecule over commercial zeolite catalysts under catalytically relevant conditions is studied using the combinatorial neutron imaging method.[4] The large interaction between neutrons and hydrogen leads to significant changes in contrast when H-containing molecules are adsorbed on the materials. This property enables the in-situ adsorption/desorption visualization, and the quantification of the hydrocarbon species adsorbed. In addition, the custom designed experimental setup used in this study allowed the simultaneous investigation of up to 69 samples.[4] For temperatures below 473 K, the observed radial diffusion profiles in most porous materials indicate that the diffusion of long chain products plays a critical role in the catalyst deactivation under typical reaction temperatures (423-523 K). Overall, the findings provide new insights on the adsorption kinetics of hydrocarbons over systems with varying porosity and pore connectivity, facilitating the design of optimized catalysts for oligomerization reactions.

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