

Analysis of alkane uptake over commercial C₁-C₄ coupling catalysts by combinatorial neutron imaging

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Today's reliance on fossil source-derived long-chain hydrocarbons, key commodity chemicals used in various end-user applications such as jet fuels, puts pressure on environmental and sustainability targets. Current promising routes for the sustainable production of these chemicals rely on the coupling of small molecules (C₁-C₄), but the catalysts employed in these transformations suffer from poor selectivity towards a single target product,^[1] as well as rapid deactivation.^[2] Herein, neutron imaging is utilized to gain understanding on the adsorption kinetics of two probe molecules, n-hexane (C₆) and n-dodecane (C₁₂), over several commercially available catalysts. The large cross section of neutron with hydrogen gives rise to strong contrast changes when H-containing molecules are adsorbed on the materials, therefore allowing the quantification of such species under *operando* conditions.^[3] Furthermore, the custom-made combinatorial setup employed for the experiments allows the simultaneous investigation of up to 69 samples under identical conditions. The results showed a strong diffusion limitation for n-dodecane over most porous materials in comparison with n-hexane, indicating that the diffusion of long chain products out of the pore network under typical reaction temperatures (473-623 K) is a crucial parameter for catalyst deactivation. These findings provide key insights on the adsorption of hydrocarbons with different lengths over systems with varying porosity and pore connectivity, enabling the future design of optimized catalysts for coupling reactions.

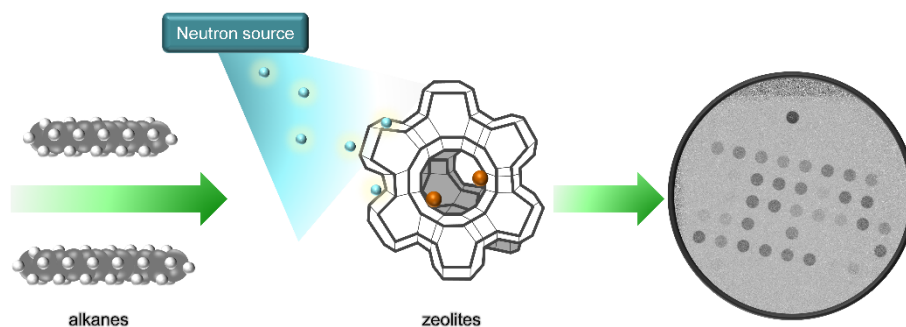


Figure 1. Schematic representation of the study.

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