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Diffusion Studies of Monobranched Alkanes in Large Crystal Zeolites Using Infrared Microscopy

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Introduction

Zeolites are promising materials for their varied applications as catalyst (supports), in hydrocarbon separation and as adsorbents. Due to their microporous structure, diffusion of molecules within the pore network can face limitations. Understanding this diffusion behavior is an integral component to further improve their application potential [1]. Microimaging using Infrared Microscopy (IRM) is a powerful tool, allowing for in situ imaging of molecule movement within a single zeolite crystal. Transport resistances can thus be investigated in greater detail than via macroscopic techniques [2]. It is the aim of this work to synthesize sufficiently large zeolite crystals for IRM (> 50 µm) and investigate the diffusion behavior of technically relevant C_6-C_8 hydrocarbons.

Materials and Methods

MFI-type zeolite crystals (> 100 µm), prepared in a hydrothermal synthesis under alkaline conditions, were used to conduct diffusion studies with monobranched alkanes via IRM. Time resolved collection of IR absorbance spectra produces uptake curves, which provide transport diffusivity values. Imaging of the uptake shows the spatial distribution of probe molecules inside the investigated crystal over time.

Results

Comparison of the diffusion experiments with monobranched alkane homologues (C_6-C_8) showed an increase of uptake and release times with increasing chain length, and an indication for the presence of a surface barrier. The difference in diffusion behavior between 2-methylpentane and 3-methylpentane was compared via small loading steps yielding their isotherms and transport diffusivities.

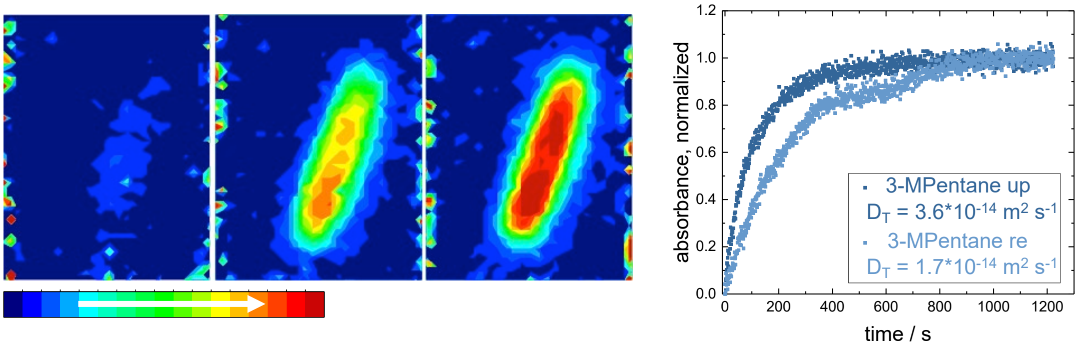

Figure 1: left: IR Imaging of uptake of 3-methylpentane inside a single silicalite-1 crystal with color bar indicating increasing probe molecule concentration, right: uptake/release curves (10^{-6} - 0.3 mbar) of 3-methylpentane and transport diffusivities.

Discussion and Conclusion

Indications for the presence of surface barriers need additional confirmation. Differences in the diffusivities of 2-methylpentane and 3-methylpentane in terms of their loading per unit cell is of further interest, as well as comparison of the experimental diffusion data with literature and simulated data.

References

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