

Transport of methyl Oleate in hierarchically structured titaniumsilicalite-1 catalysts probed by means of diffusion NMR

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Diffusion of long-chain hydrocarbons in confined environments remains in the focus of modern science. It is relevant, e.g., in the heterogeneously catalyzed oil cracking, transesterification of oils for biodiesel production or in biodiesel epoxidation. Among the major challenges associated with the utilization of nanoporous catalysts in these type of conversions are diffusion limitations. The latter occur under conditions when the reaction time scale is notably smaller than the time needed for delivery of reactants to the catalytic sites and/or product removal. The diffusion process in such case becomes dominating and determines the overall reaction rate. Thus, obtaining quantitative information on the transport characteristics of long-chain hydrocarbons confined to nanopores is vital.

In the present contribution, we demonstrate the applicability of the pulsed field gradient (PFG) NMR for probing diffusion of methyl oleate ($C_{19}H_{36}O_2$) adsorbed into the mesopore system of post-synthetically treated titanium silicalite-1 (TS-1) at room temperature. This catalyst is known to be highly selective in the liquid-phase oxidation of a wide range of hydrocarbons using aqueous H_2O_2 as the sole oxidant [1]. It is suggested that the introduction of larger (meso)pores might facilitate diffusion of methyl oleate into the crystals of hierarchically structured TS-1. In this context, the main focus of the present contribution is placed on a proof-of-principle demonstration of the direct assessment of self-diffusion coefficients of the long-chain methyl oleate adsorbed within TS-1 possessing the mesopores by means of PFG NMR [2].

References

- [1] N. Wilde, M. Pelz, S.G. Gebhardt, R. Gläser: *Highly efficient nano-sized TS-1 with micro-/mesoporosity from desilication and recrystallization for the epoxidation of biodiesel with H_2O_2* . Green Chem. **17**, 3378-3389 (2015).
- [2] J. Kärger, H. Pfeifer, W. Heink: *Principles and application of self-diffusion measurements by nuclear magnetic resonance*. Adv. Magn. Reson. **12**, 2-89 (1988).

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