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Investigations of Molecular Diffusion in FCC Catalysts

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1. Introduction

The fluid catalytic cracking (FCC) process plays a key role in the production of fuels and important raw materials from crude oil. The process of conversion of crude oil to products depends not only on the catalytic activity of the catalysts, but also on diffusion in the FCC particles, which determines the rate of mass transfer of reactants and products [1]. FCC-catalysts possess a hierarchical porous structure. Their transport properties are therefore interesting from both practical and fundamental points of view.

2. Experimental

Pulsed field gradient (PFG) NMR [2] has been applied to study molecular diffusion in industrial fluid catalytic cracking catalysts and in zeolite USY for a broad range of molecular displacements, which are essential for a detailed understanding of molecular transport in FCC catalysts, and temperatures. Typically, FCC catalysts consist of particles with sizes between 30 and 100 micrometers. These particles contain zeolite crystals and the so-called "matrix" [3], which surrounds the crystals (Fig.1).

The influence of diffusion in the zeolite micropores and in the meso- and macropores on the rate of the overall molecular transport in the FCC particles was investigated. The

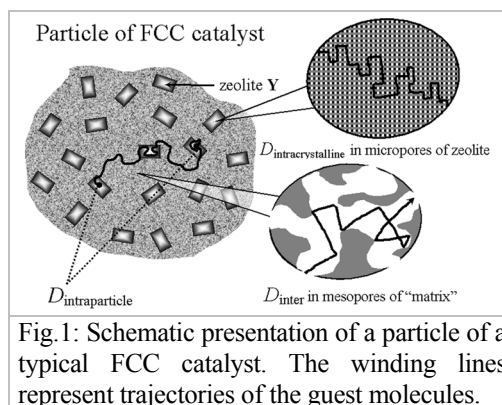


Fig.1: Schematic presentation of a particle of a typical FCC catalyst. The winding lines represent trajectories of the guest molecules.

extrapolation of the measured diffusivities associated with these two types of molecular motion for n-octane to typical FCC temperatures (Fig.2) shows that for these molecules the rate of the molecular exchange between the catalyst particles and their surroundings is primarily determined by the coefficient of intraparticle diffusion. The extrapolation to alkanes larger than n-octane shows the same result.

To confirm the relevance of this result for catalytic performance, we compared the catalytic activity of differently manufactured catalyst particles with their transport properties. In fact, we found a good correlation between the intraparticle diffusivities and the catalytic performance as assessed by the standard micro activity test (MAT) (Fig.3 and [4]).

In order to clarify the mechanism of intraparticle diffusion several FCC catalysts with identical fractions of zeolite USY, but with different properties of the meso- and macropore system in the “matrix” were investigated. The intraparticle diffusion coefficients have been measured both for varying n-octane pressure at a fixed temperature and for varying temperature for a certain molecular concentration. In this way, within the model of “long-range” (i.e. intraparticle) diffusion, the improvements in the transport properties may be referred to their microstructural origin.

All the results of the present work demonstrate the potentials of optimising FCC catalysts via an optimisation of their transport properties.

References

- [1] C.M.Bidabehere; U. Sedran, *Ind. Eng. Chem. Res.* 2001, 40, 530
- [2] P.T. Callaghan, *Principles of NMR Microscopy*; Clarendon Press: Oxford, 1991.
- [3] M.L. Ocelli, P. O'Connor, Eds. *Fluid Catalytic Cracking V. Materials and Technological Innovations*; Elsevier: Amsterdam, 2001.
- [4] P. Kortunov, S. Vasenkov, J. Kärger, et al.; *J. Chem. Mat.*; accepted 2004

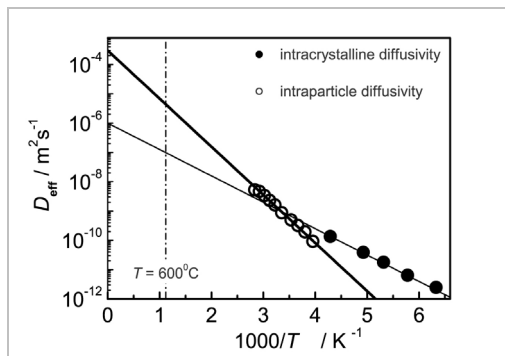


Fig.2 Temperature dependence of the intraparticle diffusivity of n-octane in an FCC catalyst and the intracrystalline diffusivity of n-octane in large crystals of USY zeolite.

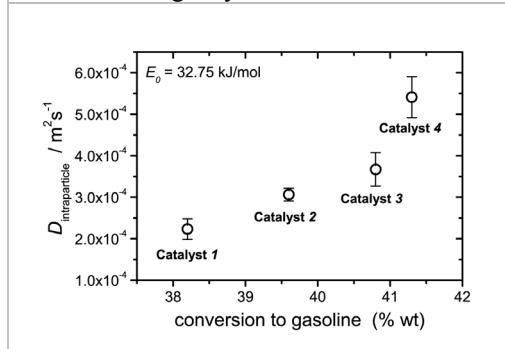


Fig.3 Correlation between the intraparticle diffusivity of n-octane and catalytic performance expressed by the oil-to-gasoline conversion for the same catalyst-to-oil ratios.