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Summary of the project goals and of the current status of the work

In this project, our intention is to find the routes of the production of fluid catalytic cracking (FCC) catalysts, which lead to improved catalytic performance due to optimization of the transport of reactants and products in these materials. The existence of about 250 refineries operating in Europe visualizes the European dimension of the project. They produce about 660 million tons per year of refined products of which gasoline production represents around 135 million tons per year with fluid catalytic cracking as a cornerstone of most refineries. Recent increases in the price of crude oil and subsequent civil unrest in countries within the EU have underscored the importance of using this resource efficiently. After the properties of the crude oil itself, the catalyst is the single most important determinant of the products that are made in the fluid catalytic cracking process.

Recent progress in the area of the pulsed field gradient technique of nuclear magnetic resonance (PFG NMR) has made possible the direct observation of molecular migration (diffusion) in microporous catalysts. In the TROCAT project this technique is used to overcome one of the main shortcomings in the optimization of FCC catalyst, i.e. the lack of the optimization with respect to the transport properties. Using PFG NMR, initially, the transport properties of the samples of the reference formulated catalyst and of the reference zeolite Y were investigated. Zeolite Y represents the most important, catalytically active part of the FCC formulated catalysts. The reference samples were chosen to closely resemble those of the catalysts currently used in the modern refineries. Further work resulted in the production of the new samples of the ultra-stabilized Y zeolite, which were prepared under various dealumination conditions. The transport properties of these samples were studied using for the most part PFG NMR. Investigations of the transport properties of the samples were complemented by the characterization of their catalytic and structural properties. The obtained results indicate that there are correlations between the catalytic performance and the transport properties. It has to be emphasized that the only difference between the new and the reference samples of ultra-stabilized Y zeolite lies in the different ultra-stabilization procedure (i.e. different temperature and duration of steaming). Hence, the ultra-stabilization presents an important route, which can be used to tune the catalytic and transport properties of zeolite Y. This route is currently further explored. The future work in this direction was made easier by the recent breakthrough in the synthesis of large crystals of zeolite Y by Universität Stittgart. The synthesis of this zeolite makes possible the unrestricted measurements of intracrystalline diffusivities using PFG NMR.

Our data suggest that for relatively small molecules ($\sim C_{10}$) the rate of molecular exchange between the catalyst particles and their surroundings may be influenced to a great extent by the intracrystalline diffusivity (i.e. diffusivity in zeolite crystals). At the same time, for large molecules this rate is primarily determined by the intraparticle diffusion coefficient (i.e. diffusivity in catalyst particles) and to a much smaller extent by the intracrystalline diffusivity. In response to this result the study of the correlations between such particle properties

as macroporosity and the macropore size distribution, which affect the intraparticle diffusivities, on one hand, and the catalytic performance of these particles, on the other hand has been carried out. To this end several catalyst samples containing the same amounts of the same zeolite Y but having different intraparticle morphology were manufactured and investigated. The molecular simulations have been performed in order to help to understand an influence of the morphology of catalyst particles on the intraparticle transport properties. The results obtained show that the samples with higher catalytic activity also reveal larger intraparticle diffusivity. The catalyst optimization route leading to higher intraparticle diffusivities is considered to be especially promising at this point. The high potentials of this route are demonstrated by the preparation of the new catalyst samples GRACE 4 and GRACE 5 showing better catalytic performance than the reference GRACE 1 sample.

The ultimate goal of the project is to improve the FCC catalyst by optimizing its transport properties. The practical result of this optimization is an increase in efficiency of production of transport fuels and lower undesired by-products such as coke and bottoms. This optimization would have the practical effects of conserving crude oil. It would also lead to the reduction of pollutant emissions resulting in a cleaner environment.