Inorganic Materials & Catalysis

Research Project - Emiel Hensen/Nikolay Kosinov/Yujie Liu



Dehydroaromatization of methane over Mo/ZSM-5 catalysts

Non-oxidative methane dehydroaromatization (MDA) is a promising technology to directly convert methane – main component of nature gas - into liquid aromatic hydrocarbons and hydrogen. Zeolite based Mo/ZSM-5 composite is a benchmark catalyst for the MDA process, allowing 10-12% methane conversion with a benzene selectivity of 60-80% at 700 °C, as reported in the literature [1].

$6 CH_4 \rightleftharpoons C_6H_6 + 9 H_2$

To make MDA commercially applicable one major challenge has to be overcome – rapid and inevitable deactivation of the catalyst [2]. During the MDA reaction, carbonaceous deposits are quickly formed in large amounts, and then block the active sites and the zeolite micropores and lead to a complete catalyst deactivation. The deactivation problem has not yet been solved, although Mo/ZSM-5 has been studied for more than 25 years. The main reason for that is limited understanding of the methane conversion mechanism and the structure of the working catalyst. This project focuses on gaining a deeper molecular insight into the mechanism of MDA reaction.

Techniques used:

Ar adsorption, H₂-TPR, XRD, TEM, EDX, XPS, FT-IR, EXAFS, XANES, MAS-NMR, XRD

Possible projects:

- Synthesis and characterization of welldefined Mo/HZSM-5 catalysts and testing of their catalytic performance in MDA reaction
- Determination of the structure of the hydrocarbon pool molecules inside the pores of Mo/HZSM-5 catalysts by a set of operando spectroscopy techniques
- Establishing a kinetic model of the MDA process with the help of isotope labelling kinetic techniques
- Designing the second generation of MDA catalysts



Figure 1. Schematic diagram of MDA reaction



Figure 2. Dispersion of Mo species on ZSM-5 catalysts with different Mo loading ^[2]



Figure 3. Proposed mechanism of methane aromatization on Mo/zeolite catalysts ^[3]

For further information

Emiel Hensen (Helix, STW 3.33), Tel 5178, <u>e.j.m.hensen@tue.nl</u> Nikolay Kosinov (Helix STW 3.27), Tel 8156, <u>N.A.Kosinov@tue.nl</u> Yujie Liu (Helix STW 3.31), Tel 6192, y.liu7@tue.nl

References:

- [1] Z.R. Ismagilov, E.V. Matus, L.T. Tsikoza, Energ. Environ. Sci. 1 (2008) 526-541.
- [2] N. Kosinov, F.J.A.G. Coumans, E.J.M. Hensen et al., J. Catal. 346 (2017) 125-133.
- [3] N. Kosinov, A. Wijpkema, E.J.M. Hensen et al., Angew. Chem. Int. Ed. 57 (2018) 1016-1020.