120a Diffusion of C7 Hydrocarbons in Mesostructured Zeolitic Ul-Zsm-5 Materials

Mladen Eic, Hoang Vinh Thang, Do Trong On, Qinglin Huang, and Serge Kaliaguine Mesoporous UL-ZSM-5 materials (Si/Al = 50) have zeolitic structure in the form of nano-particles intergrown in the walls of the amorphous wormhole-like aluminosilicate mesopores of Al-Meso-50, which was used as a precursor in the synthesis. The diffusion of two C7 hydrocarbons, i.e., n-heptane and toluene in four UL-ZSM-5 materials with different microporosities, mesoporosities and crystallinities, in addition to the precursor (Al-Meso-50) and a reference MFI zeolite sample, were investigated by the Zero Length Column (ZLC) method. Effective diffusivity values of n-heptane in UL-ZSM-5 samples were observed to be lower in comparison to toluene that has a larger kinetic diameter, while diffusion activation energies were found to be about two times higher. A theoretical model taking into consideration the combination of mesopore diffusion due to a surface slip in the main pores with an activated surface/micropore diffusion in the intrawalls of the bi-porous structure was proposed, and employed to interpret the experimental ZLC results. Classical Knudsen type of diffusion, that typicaly overpredicts the transport (diffusion) coefficient in the mesopores by several orders of magnitude, was replaced by an activated surface slip type of diffusion mechanism. The transport of n-heptane in UL-ZSM-5 materials was found to be mainly controlled by mesopore diffusion in the main channel structure, while that of toluene was dominated by intrawall diffusion process involving both external surface areas and micropores of the ZSM-5 nano-crystals. The main mesopore channel structure appears to appreciably contribute in facilitating the overall mass transport.