Para-Xylene Synthesis by an In-situ Methylation of Toluene with Syngas over Bifunctional Catalysts

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Para-Xylene is an important raw material in the petrochemical industry for terephthalate and polyester. The direct conversion of toluene with syngas (CO + H2) over bifunctional catalysts for the selective formation of para-xylene is a challenging process. In this study, we investigated an in-situ methylation of toluene with syngas over bifunctional mixtures of modified HZSM-5 and methanol synthesis catalysts in comparison to the conventional MeOH/Tol methylation process. The in-situ methylation was studied in a fixed bed downflow reactor in the temperature range of 400-500℃ under the total pressure of 460 psig. The in-situ methylation exhibited many catalytic synergies in terms of xylene yield as well as CO and toluene conversion over monofunctional counter parts and MeOH/Tol methylation process. The effects of ratio of catalytic functions and modification of HZSM-5 on the total xylene yield and para-selectivity in the in-situ methylation were studied in detail. Catalysts were characterized by using X-ray diffraction (XRD), field emission scanning electron microscope (FE-SEM) with EDS, HRTEM, temperature programmed desorption of ammonia and DTBPy (di-tert-butyl pyridine), etc. The reaction products were analyzed by using GC with a thermal conductivity detector (TCD, gas product) and a flame ionization detector (FID, liquid product).