Bifunctional Catalysts of Silicalite-1/H-ZSM-5 and Cr₂O₃/ZnO for Para-Selective in-Situ Methylation of Toluene with Syngas

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In-situ methylation, a chain reaction that includes methanol synthesis and toluene methylation, could be one route of converting syngas into liquid chemicals. Alkylaromatics can be directly synthesized by reacting aromatic compound such as toluene with syngas (CO + H2) at alkylation conditions in the presence of zeolite and methanol synthesis catalyst. In this study, an in-situ alkylation of toluene with syngas was studied over bifunctional mixture of silicalite-1/H-ZSM-5 shell/core structure and metallic Cr2O3/ZnO catalysts for the selective formation of para-Xylene. The in-situ methylation over bifunctional catalyst showed catalytic synergies in terms of CO/H2 conversion of syngas, toluene conversion and xylene yield compared to the corresponding monofunctional catalyt. 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).