

Evaluation of Equilibrium Displacement in the *in situ* Methylation of Toluene with Syngas over Bifunctional Catalysts

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Many catalytic systems are controlled by equilibrium conversions and thus yield limited per-pass performances. The equilibrium limitation can be partially circumvented by accelerating the desired reaction via physical separation methods, reaction system and catalyst designs etc. Methanol synthesis from syngas and para-xylene selectivity in toluene methylation are typical examples of equilibrium controlled reactions. Herein, the direct conversion of syngas (CO+H<sub>2</sub>) and toluene into para-xylene was studied over bifunctional catalysts under a moderate total pressure of 460 psig. In the *in situ* methylation of toluene with syngas, a high per-pass CO conversion beyond the equilibrium limitation inherent in methanol synthesis was observed. The equilibrium displacement achieved in the *in situ* methylation over bifunctional catalyst was further elucidated by monofunctional model reactions (benzene and toluene methylation with methanol over HZSM-5). By employing modified HZSM-5 in the *in situ* methylation, the para-xylene selectivity exceeding the equilibrium composition was also achieved.