ABSTRACT OF PhD THESIS OF SACHIN TOMAR

Decomposition of Sulfur Trioxide over Mixed Metal Oxide Catalysts in the Sulfur–Iodine Cycle for Hydrogen Production

The sulfur–iodine (S–I) cycle is one of the promising thermochemical methods for water–to–hydrogen conversion in an efficient and eco–friendly manner. SO_3 decomposition is the most endothermic reaction of the S–I cycle. Some of the major challenges in the SO_3 decomposition step of the S–I cycle are sintering, long term stability and cost of the catalytic system. Along with the better catalytic design, understanding of the kinetics of the catalytic decomposition is essential for the implementation of the process at a large scale. Reported literature primarily focused on the power–law type models. The literature till date is lacking in the heterogeneous kinetic modeling and validation of the models with the experimental studies of the reaction. Furthermore, separation of the acid mixture ($HI–H_2O–I_2$) is a matter of concern in the S–I process. There is presence of $HI–H_2O–I_2$ (HI_x) phase in sulfuric acid which is the feed for the SO_3 decomposition reaction. The impurities in sulfuric acid have a remarkable influence on the catalytic performance in the SO_3 decomposition reaction. The practical aspect on how the iodine–based impurities could affect catalytic activity has been scarcely addressed until now. From the commercial operation point of view, the severe impact of the feed impurities on the catalytic performance necessitates a highly active and stable catalytic system for SO_3 decomposition in the integrated S–I process.

Hence, there is a need for cost effective, highly active as well as stable catalysts with the right choice of supports in this high temperature endothermic reaction which is important for scale-up of the process. Copper ferrite ($CuFe_2O_4$) was dispersed over the suitable supports and characterized by different physicochemical techniques. The catalysts were activity tested and compared in high temperature (800–900 ˚C) endothermic SO_3 decomposition reaction in the S–I cycle for hydrogen production. The kinetic modeling over the synthesized catalysts was studied. Furthermore, the effect of the feed impurities on the catalytic performance was investigated.