Microkinetic modling of DME synthesis from methanol over a H-zeolite catalyst

박종민, 조지영, 박명준[1], 이원보†
서울대학교; [1]아주대학교
(wblee@snu.ac.kr†)

In this study, microkinetic modeling was conducted for dimethyl ether (DME) synthesis from methanol on basis of computational chemistry. The possible elementary-step reactions of the methanol dehydration reaction including the associative and dissociative pathways were considered for DME synthesis from methanol over a H-zeolite catalyst. Reaction energetics and structures of the reaction intermediates and transition states were calculated by using computational chemistry such as the second-order Møller-Plesset perturbation theory (MP2). Using the results, the activation energies were applied to the microkinetic model, and the pre-exponential factors were estimated by fitting the experimental data, increasing the reliability of our model. Using the parameter-fitted microkinetic model, the dominant reaction pathway was elucidated on basis of relative rates of the elementary steps, and the rate-determining steps were suggested. In conclusion, our analysis using both computational chemistry and microkinetic model could provide valuable information on the reaction mechanisms and kinetics.