A microkinetic model for methanol synthesis from syngas over Cu-based catalyst

<u>박종민</u>, 조지영, 박명준[1], 이용규, 이원보[†]

서울대학교; [1]아주대학교

(wblee@snu.ac.kr[†])

In this study, a practical and computationally cost-effective microkinetic model was developed for the methanol synthesis from syngas over Cu-based catalyst. The reaction mechanisms consisted of CO and CO_2 hydrogenations and water-gas shift (WGS) reaction were considered. Density functional theory (DFT) which could calculate the enthalpies and adsorption energies of gas and surface intermediates and the semi-empirical unity bond index-quadratic exponential (UBI-QEP) method were combined to determine the heat of adsorption and activation energies. Pre-exponential factors were estimated by fitting experimental data, reducing the computational burden by excluding the calculation procedure of vibrational frequencies of the reaction species and partition functions. Based on relative reaction rates of the reaction steps, the most plausible reaction pathways for the methanol synthesis were found, and the rate determining surface reaction was suggested by the degree of rate control. Proper operating conditions were also proposed by evaluating the effects of temperature, pressure and the H2 fraction in the feed on the methanol synthesis rate.