Kinetic Modeling of Naphtha Cracking Reaction based on Mechanistic Reaction Pathway

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Naphtha-to-Olefin (NTO) reaction by catalytic cracking is one of the ways to product ethylene and propylene, which is basic materials in the petrochemical industry. NTO reaction mechanism is complex, and many reaction mechanisms have been studied. There are three types of model for reaction mechanisms. Lumped model is lumping hydrocarbons that have similar properties such as paraffins, olefins and aromatics. Molecular model treats hydrocarbon molecules such as methane, ethane, and benzene. Mechanistic model considers radical or carbenium ion on the catalyst surface as well as hydrocarbon molecules. The complexity of model increases from the lumped model to the mechanistic model, and the computational load as well. But, the intrinsic reaction rate can be obtained in the mechanistic model. In this study, we developed a kinetic model based on the mechanistic model. It consisted of 1454 elementary reaction and 192 reaction components. To construct mechanistic model, single-event approach was used, which is derived from the transition state theory (TST). As a validation, we compared the prediction of model on product yield with experimental data, which was given by KRICT.