Efficient parameter estimation for microkinetic reaction modeling of catalytic heavy-naphtha cracking process

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Catalytic naphtha cracking (CNC) process that produces olefins has been studied to improve efficiency. The yield of CNC process is 10% higher than conventional cracking process, and CNC demands lower temperature (500~650℃) than the conventional cracking temperature (800~900℃) due to performance of a solid acid catalyst. It is considerably difficult that estimate parameters accurately in a complex model. Therefore, to develop commercial scale CNC process, kinetic modeling of CNC process is crucial. In this study, Parameters are estimated in two step, Step 1 : Approach to the global optimum via Genetic Algorithm (GA), Step 2 : Find the global optimum via Levenberg-Marquardt (LM) method starting from the initial point found in step 1. The advantages of this 2 step procedure are that, we can avoid the possibility of premature convergence using GA, and we can fine tune the optimum using LM method. Consequently, the parameters can be accurately estimated with the experimental data.