Kinetic Modeling of Acidity-Activity Relationship for Ethylene Oligomerization and Aromatization Over ZSM-5 Zeolites

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May 5, 2020

Abstract

The ethylene oligomerization and aromatization reaction kinetics on ZSM-5 with different Si/Al ratio was modeled by the single-event concept combined with the Brönsted kinetic model for establishing a quantitative acidity-activity relationship. The NH3 desorption activation energy is related to the reaction activation energy and de/protonation heat based on the linear free energy theory by introducing γ, δ as the kinetic parameters of reaction sensitivity to the acid strength. Total 36 parameters in the subtype elementary step level were estimated for each kinetic model. The hybrid genetic optimization algorithm was generated to obtain the kinetic model parameters, which can efficiently and accurately fit the change of product distribution of for 3 three catalysts within C8 hydrocarbon in the reaction network. The performance of the kinetic modeling is confirmed by experimental data. The regressed kinetic modeling can predict the influence of zeolite with same topology and different acidity on product distribution.

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