Title: Deconvolution of Polymerization Kinetics and Polymer Microstructures for Ethylene/1-Olefin Copolymers Produced from Two-Reactor System

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Abstract:

Note: maximum length of 400 words.
The production of ethylene/1-olefin copolymers in two-reactor system has received increasing attention because it can produce polymers with a wide range of characteristics and applications. The system allows production flexibility by adjusting different feeding conditions and operating conditions in each reactor. Ethylene/1-olefin copolymers in industrial production required catalysts, typically Ziegler-Natta catalysts, which are multiple-site catalysts. This catalyst type produces polymers with board chain microstructures because of different kinetic parameters in each site type. Understanding the effect of polymerization conditions on chain microstructures of polymers made on each site type can help control desired polymer structures and their properties. Besides, kinetic parameters and the microstructures on each site type are related to polymerization rate (R_p) and the cumulative polymer yield during polymerization (Q_p). Various of R_p and Q_p in each site type also affect many important microstructures, including molecular weight distribution (MWD), chemical composition distribution (CCD), and comonomer sequence length distribution (triads distribution). These microstructures also control mechanical and rheological characteristics of ethylene/1-olefin copolymers (e.g., tensile strength, machinability, and elongation). However, there is currently no characterization technique that can directly measure kinetic parameters and microstructures of each site type from the experiment.

Deconvolution is the methodology developed to estimate the number of site-type and kinetic parameters of each site type by performing parameter estimation to minimize the sum of the squares of differences between experimental and experimental and/or model data. In the literature, the methods are available but still largely limited to a simple single reactor system. This work aimed to develop the deconvolution method to estimate kinetic parameters of ethylene/1-olefin copolymers produced from multiple site-type catalysts in a two-reactor system. The deconvolution is based on MWD, CCD, triads distribution, R_p and Q_p. The developed model was validated by comparing the deconvolution results with the model data. In addition, deconvolution method for two-reactor systems can accurately identify the number of site types in each reactor and adequately estimate the kinetic parameters of each site type and mass fraction of polymers produced from each reactor.