Suwicha Sottisakul 2014: Mathematical Modeling of Chain Microstructures of Olefin Block Copolymers. Master of Engineering (Chemical Engineering), Major Field: Chemical Engineering, Department of Chemical Engineering. Thesis Advisor: Assistant Professor Siripon Anantawaraskul, Ph.D. 90 pages.

Linear olefin block copolymers (OBCs) produced from chain shuttling polymerization posseses statistical multi-block structure, leading to the unique thermoelastic properties compared to the conventional ethylene/1-olefin copolymers. In this research, the effect of operating conditions of chain shuttling polymerization on the microstructures of OBC were studied. Four main operating condition parameters consisting of catalyst selection probability, chain propagation probability, chain shuttling probability, and chain termination properbility were considered.

The investigated chain microstructures included longest ethylene sequence distribution and chemical composition distribution of OBCs, which were obtained by using the Monte Carlo simulation. Moreover, the mathematical equations based on statistical and probabilistic theory were developed to describe chemical composition distribution of OBCs and used to comfirm the results obtained from Monte Carlo simulation.

Furthermore, those results were compared with simulated TREF profile from TREF model. It was found that the simulated TREF profile cannot directly reflect the complicated microstructures of olefin block copolymers.

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