# Chemical Composition Distribution of Linear Olefin Block Copolymer: Theoretical Analysis and Monte Carlo Simulation.

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Linear olefin block copolymers (OBCs) produced from chain shuttling polymerization processes have thermoplastic elastomer behavior compared to those of conventional random copolymers due to the unique statistical multi-block structures. Chemical composition distribution (CCD), which describe how comonomer distribution among copolymer chains, is one of the important chain microstructure information for copolymers because it could significantly influence the end-use physical properties. Previously, mathematical expressions for describing CCD of OBCs have not been reported.

In this research, probabilistic and statistical analysis was used to develop mathematical equations for describing chain microstructures of OBCs in term of chemical composition distribution (CCD), distribution of the number of blocks, distribution of block length, and distribution of chain length. CCD results obtained from derived mathematical equations were validated with those obtained from Monte Carlo simulation. Effects of operating conditions (in terms of catalyst selection probability, chain propagation probability, chain shuttling probability, and chain termination probability) on CCD and other chain microstructures were investigated.

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