Title: Chain Microstructures of Olefin Block Copolymers (OBCs): Theoretical Model and Its Applications in Materials Design

Main Author:

Name:	Tamaned Chayrattanaroj
Organization:	Department of Chemical Engineering, Faculty of Engineering, Kasetsart University
Country:	Thailand

Co-Authors:

Co-author 1:	Sompob Buaparungsri
Organization:	Department of Chemical Engineering, Faculty of Engineering, Kasetsart University
Country:	Thailand
Co-author 2:	Suwicha Sottesakul
Organization:	Department of Chemical Engineering, Faculty of Engineering, Kasetsart University
Country:	Thailand
Co-author 3:	Poramet Buakrong
Organization:	Department of Chemical Engineering, Faculty of Engineering, Kasetsart University
Country:	Thailand
Co-author 4:	Siripon Anantawaraskul*
Organization:	Department of Chemical Engineering, Faculty of Engineering, Kasetsart University
Country:	Thailand
Co-author 5:	João B. P. Soares
Organization:	Department of Chemical and Materials Engineering, University of Alberta
Country:	Canada

References:

Reference 1:	Arriola DJ, Carnahan EM, Hustad PD, Kuhlman RL, Wenzel TT. Science. 2006 May 5;312(5774):714-9.
Reference 2:	Wenzel TT, Arriola DJ, Carnahan EM, Hustad PD, Kuhlman RL. In Metal Catalysts in Olefin Polymerization 2009 (pp. 65-104).
Reference 3:	M. Zhang, T. W. Karjala, P. Jain, Ind. Eng. Chem. Res. 2010, 49, 17, 8135–8146
Reference 4:	S. Anantawaraskul, P. Somnukguande, J. B. P. Soares, Macromol. Symp. 2009, 282, 205.
Reference 5:	S. Anantawaraskul, P. Somnukguande, J. B. P. Soares, Macromol. Symp. 2012, 312, 167.
Reference 6:	T. Tongtummachat, S. Anantawaraskul, J. B. P. Soares, Macromol. Theory Simul. 2017, 26, 1700012.
Reference 7:	T. Tongtummachat, S. Anantawaraskul, J. B. P. Soares, Macromol. React. Eng. 2018, 12, 1800021.
Reference 8:	
Reference 9:	
Reference 10:	
Reference 11:	
Reference 12:	

Images:

Abstract:

Discovering the chain-shuttling polymerization system allows us to tailor-make olefin block copolymers (OBCs), a new type of thermoplastic elastomer (TPA) with unique properties due to their alternating multiblock structures. This system consists of two catalysts with different reactivity ratios and a chain-shuttling agent (CSA). Polymers with low comonomer incorporation ("hard-blocks") are produced by one of the catalysts, while polymers with higher comonomer incorporation ("soft-blocks") are produced by the other. A multiblock structure alternating between hard and soft blocks is produced by adding CSA to shuttle growing polymer chains back and forth between both catalysts.

The analysis of OBC chain microstructures can be accomplished using several techniques, such as GPC, TREF, and CRYSTAF. However, the specific OBC chain microstructures, such as the distribution of the number of blocks per chain, the distribution of the length of the hard and soft blocks, and the distribution of chains with a particular composition, cannot be directly probed by these characterization techniques because they can only measure the overall chain microstructures.

In this work, mathematical equations were developed to describe OBC microstructures. The Monte Carlo model was used to validate the proposed model. The equations can describe average features of microstructures, molecular weight distributions (MWD), and chemical composition distributions (CCD) well. They can also explain how reaction probabilities (i.e., catalyst selection, propagation, chain-shuttling, and termination probabilities) affect microstructures. Most importantly, CCD multi-modality criterion for OBCs was developed for further materials design by controlling catalyst ratio and comonomer incorporation in each catalyst.