Ekaphol Siriwongsarn 2012: Simulation of Temperature Rising Elution Fractionation (TREF) Using Population Balance and Kinetic Models. Master of Engineering (Chemical Engineering), Major Field: Chemical Engineering, Department of Chemical Engineering. Thesis Advisor: Assistant Professor Siripon Anantawaraskul, Ph.D. 84 pages.

Temperature rising elution fractionation (Tref) is a characterization technique widely used for estimating chemical composition distribution (CCD) of semi-crystalline copolymers. To elucidate the quantitative fractionation mechanism and accurately interpret Tref profiles, several Tref models have been proposed. However, all previous Tref models are based on the equilibrium fractionation and, therefore, cannot describe the important kinetics roles in Tref analysis observed in experiments.

In this investigation, a new mathematical model of Tref was developed based on the population balance concept with the incorporation of kinetic models describing crystallization and dissolution during the fractionation process, which are ignored in all previous Tref models. The results showed that the proposed Tref model can describe the effects of molecular weight, comonomer content, and operating conditions (i.e., cooling rate, heating rate, and solvent flow rate) on Tref profiles of ethylene homopolymers and ethylene/1-olefin copolymers observed from experiments very well. The simulated Tref calibration curves based on the proposed model were also investigated as an efficient alternative to the experimental Tref calibration curves, which is often, required the tedious process.

Moreover, Monte Carlo simulation and the modified Tref model are used to predict Tref profiles of polymers with more complex microstructures (i.e., polymer blend and linear olefin block copolymers). The modified Tref model was found to be useful to help identify the link between Tref profiles and chain microstructures of polymers.

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