

Thtitporn Sooksod 2010: Simulation of Morphological Development during Polymer Crystallization in a Temperature Gradient. Master of Engineering (Chemical Engineering), Major Field: Chemical Engineering, Department of Chemical Engineering. Thesis Advisor: Assistant Professor Siripon Anantawaraskul, Ph.D. 114 pages.

Polymer crystallization in the industrial process mostly occurs in temperature gradient. This research investigated crystallization simulation of syndiotactic polypropylene in 2 dimensions in a temperature gradient, which affects crystallization kinetics and morphological development during polymer crystallization. Crystallization kinetics obtained from simulation was found to be in a good agreement with those obtained from experiments, confirming the validity of the proposed simulation approach. It was found that temperature gradient affected nucleation density and position of nuclei. Most of nuclei occurred in the low temperature area. It also affected the spherulite shape, distorting to an elliptical shape. The shape is depended on position of nuclei at the considered temperature period. For crystallization in temperature range between 40°C and 100°C (heterogeneous nucleation) and between 10°C and 40°C (homogeneous nucleation), it was found that temperature gradient affect crystallization kinetics and morphological development. Effect of temperature gradient on nucleation density, distribution of nuclei position and growth rate must be considered. The study found that the average of Avrami crystallization rate constants can be used to indicate crystallization kinetic rate, especially at the early of crystallization.

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