CONCLUSION

A stochastic simulation, which considers both nucleation and growth process during polymer crystallization, was developed to describe crystallization kinetics and morphological development. The effect of number of predetermined nuclei, growth rate, and crystallization temperature on crystallization kinetics and detailed morphological development during isothermal crystallization of polymer was investigated.

Effect of Number of Predetermined and Growth Rate

The simulated crystallization kinetics results are in a good agreement with results from the theoretical Avrami equation. It was found that number of predetermined nuclei has a significant impact on both crystallization kinetics and polymer morphology. An increase in the number of predetermined nuclei fastens a crystallization process by speeding up the impingement phenomena and increasing the level of impingement. A growth rate has a stronger impact on crystallization kinetics, but it only helps speed up the impingement phenomena without increasing the level of impingement. Although a growth rate influences an average spherulite size and distribution of spherulite size during the crystallization, it has no effect on a final morphology.

Effect of Crystallization Temperature

The effect of crystallization temperature on crystallization kinetics and detailed morphological development during isothermal crystallization of polymer was investigated. The simulation procedure based upon experimental data of syndiotactic polypropylene reported in the literature. The simulated crystallization kinetics results are in a good agreement with results from the theoretical Avrami equation

It was found that crystallization temperature has a significant impact on both crystallization kinetics and polymer morphology. A decrease in the crystallization

temperature from 90^{o}C to 70^{o}C cause fastens a crystallization process induced by increase in both concentration of predetermined nuclei and spherulite growth rate, speeding up the impingement phenomena and increasing the level of impingement. The competing effect of concentration of predetermined nuclei and spherulite growth rate can be observed at the crystallization temperature lower than 70^{o}C.

A growth rate has a stronger impact on crystallization kinetics, but it only helps speed up the impingement phenomena without increasing the level of impingement. Although a growth rate influences an average spherulite size and distribution of spherulite size during the crystallization, it has no effect on a final morphology.

The use of experimental input data for syndiotactic polypropylene and the subsequence comparison with experimental results allowed us to conduct a quantitative validation of the model. The good agreement between simulated and experimental results showed that the model is capable of correctly reproducing the kinetics for syndiotactic polypropylene only. To modify the model for other polymer, the experimental data of growth rate (G) and number of predetermined nuclei (N) are required in the program.