Nutshera Kitthitanesuan 2008: A Study on Size and Shape of Polymer Molecules with Complex Topology using Monte Carlo Simulation. Master of Engineering (Chemical Engineering), Major Field: Chemical Engineering, Department of Chemical Engineering. Thesis Advisor: Assistant Professor Siripon Anantawaraskul, Ph.D. 59 pages.

This research work studied size, shape, and chain conformation of polymer molecules with complex topology using Monte Carlo simulation with biased self-avoiding walk (SAW) model in a three-dimension cubic lattice. 3 cases were considered. In the first case, the characteristics of semi-flexible di-block and multi-block copolymer were investigated. The mathematic equations for describing effect of segment sequences on the mean square radius of gyration $<R_g^2>$ and the mean square end-to-end distance $<R_e^2>$ were developed. It was found that the mathematic equations well explain the results from Monte Carlo simulation. In the second case, the characteristics of linear homopolymer with Flory's molecular weight distribution were studied. It was found that the relationship between the average size and the average number of segment obtained from Monte Carlo simulation agree well with the theoretical predictions. The molecular weight distribution is broadened with the increase in the average number of segment. In the last case, the characteristics of uniform star homopolymers were studied. The investigated numbers of segments are 60, 120, 180, 240, and 300 and the investigated numbers of arms equal to 2, 3, 4, 5, and 6. It was found that the size of uniform star homopolymers increases with the number of segment, but it decreases with the increase in the number of arms. Moreover, it was found that the g factors of polymers with the same topology are constant, independent of the number of segments. The g factor from Monte Carlo simulation with biased self-avoiding walk (SAW) model is close to the g factor obtained from theoretical analysis of random walk (RW) model.

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