

Abstract

In this work we study properties of branched polymers in a good solvent. We focus on problematic related to the size exclusion chromatography and predicting elution behavior of randomly branched polymers. We developed a software for generating self-avoiding walks (SAW) of any given non-looping architecture on a cubic lattice using Monte Carlo (MC) simulation and validate its reliability by presenting the scaling of different architectures: linear, 3-arm star and 6-arm star and asymmetric star. We calculate distribution coefficients and calibration curves for size exclusion chromatography for various architectures to validate that the hydrodynamic radius is more suitable for predicting elution volume than the radius of gyration. Then we propose a new method for, although approximate, a very fast estimation of radius of gyration and hydrodynamic radius for different architecture using a graph method. It is done by comparing MC results with results obtained from graph theory. Then we introduce a correction to graph-theory results to fit the MC. At the end we present depletion layer calculation from MC and self-consistent field (SCF) method for polymers and their comparison. We show how calculation of depletion layer using SCF can be improved to get significantly better agreement with MC results.