Abstract

The presented bachelor thesis deals with the study of the conformational behavior of polymer dendrimers in aqueous solutions. The polymer solution was simulated via dissipative particle dynamics. All simulations were performed using the simulation software DL_MESO. The own software was written for the generation of input files and for the post processing of the simulation results. The proper function and proper setting of simulation parameters was verified by a parametric study of the infinitely dilute solutions of dendrimers in a good solvent. The obtained scaling exponent of the gyration radius is in agreement with the published data. Moreover, the conformational behavior of homopolymer and copolymer dendrimers was compared.

Keywords: Computer simulations, dissipative particle dynamics, dendrimer, conformational behavior, aqueous solutions, branched polymer