

Abstract

The presented diploma thesis is devoted to computer simulations of the interactions of amphiphilic copolymer dendrimers in diluted solutions by means of the dissipative particle dynamics. We focus mainly on the solubilization of low molar compounds in the solvophobic part of dendrimer in selective solvents. Studied copolymer dendrimers have two inner solvophobic generations and one or two outer solvophilic generations. The solubilized compounds are solvophobic monomer and tetramers.

In the first part of the diploma thesis, fundamental information about dendrimers is presented and the principles of the applied simulation methods are explained together with the definition of used quantities.

The second part is devoted to the study of solvophobic low molar compound solubilization in the copolymer dendrimer. The most important trends concerning the size and inner structure of aggregates are analysed and discussed. We have found that the preferential attraction between solvophobic compound and solvophobic dendrimer core is essential for a sufficient solubilization. The solubilization of low molar compound was studied as function of the attractive interaction and concentration of monomers, resp. tetramers, and the copolymer dendrimer architecture and composition.

We conclude that the most prospective systems from the application point of view are dendrimers with relatively long spacer and large enough outer solvophilic shell. The solvophobic compounds with the attraction to the dendrimer core are more proper than the compounds without the attraction. Simultaneously the oligomer chains promote the solubilization.

Keywords: Dissipative particle dynamics, computer simulations, amphiphilic, copolymers, dendrimers, selective solvent, solubilization, conformational behavior