Dissipative particle dynamics study of the amphiphilic functionalized polymer dendrimers and their interactions with the linear block copolymers in dilute solutions

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Great application potential of polymer dendrimers was recognized immediately after the first synthesis of this type of polymers as these three dimensional nano-sized globular macromolecules have well defined architectures, shapes and sizes. Simultaneously, dendrimers offer a number of possibilities how to modify and control their properties. The low molar agents may be encapsulated in to the interior of dendrimers or attached onto dendrimer surface. Furthermore, dendrimer can be tailored for specific needs by the functional groups. Functional peripheral groups can improve the solubility of dendrimer and/or enhance the solubility of low molar agents. The functionalized branching points with preferential interaction with low molar compound can work as "condensation centers" and enlarge the amount of encapsulated agents. In the case of copolymer dendrimer, the core may be also tailored as nanocontainer for specific drugs or pollutants. Local or global bifunctionalization enables two or more functions being present in one dendrimer molecule and is very important for so called "smart" applications.

Recent developments in synthesis provided a large variety of functionalized dendrimer structures and nowadays extensive experimental research of such systems is running. The computer simulations of these systems are very desirable because they elucidate the complex behavior of dendrimer solution from the thermodynamic point of view and so represent helpful assistance for experimental work.

We studied the solubilization of low molar compound in functionalized amphiphilic polymer dendrimer in the dilute solutions by means of dissipative particle dynamics. We focused on the better understanding of the relation between the amount of solubilized compounds and the types, positions and interactions of functional groups on the one side and the conformational behavior of polymer dendrimer and the architecture of obtained nanostructures on the second side.

Acknowledgements This work was funded by Czech Science Foundation Grant P106–12–0143 and by Grant 422216 of the Grant Agency of the Charles University.