PHASE DIAGRAMS OF AMPHIPHILIC P-GRAFT-H HOMOPOLYMER SOLUTIONS: MESOSCOPIC COMPUTER SIMULATION AND THEORY

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Phase diagrams of P-graft-H homopolymer dilute solutions were evaluated by means of dissipative particle dynamics simulations [1] with explicit solvent and analytical theory [2]. As an example of such system can be a solution of single stranded DNA molecules with hydrophilic sugar-phosphate backbone and hydrophobic bases.

During the equilibration process chains of amphiphilic macromolecules tend to aggregate into various structures such as spherical globule, onion-like and vesicles particles, cylinder and necklace formations. Type of self-assembling structure depends on solvent quality and degree of incompatibility of polar and hydrophobic groups which were controlled by repulsion parameters of soft-core potentials. Dependence of structure type on bond stiffness and length of chains were also investigated.

The diagrams were constructed based on shape factor and aggregation number calculations and evaluated by the analytical theory, wherein the type of structure is determined by bulk and surface effects interplay.

References:
[1] *Groot R. D., Warren P. B*. J. Chem. Phys. **107**, 4423 (1997).
[2] *Larin D.E., Glagoleva A. A., Govorun E. N., Vasilevskaya V.V.* Polymer. **146**, 230-241 (2018).

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