Krajowa Konferencja Zastosowań Matematyki w Biologii i Medycynie

Sandomierz, 5th–9th September 2016

POLYMERIZATION OF COMPLEX MACROMOLECULES USING ATRP METHOD — COMPUTER SIMULATION STUDIES

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ABSTRACT

Technological progress in biology and medicine requires new advanced polymeric materials with precisely defined complex architecture. Synthesis of such materials is challenging, and requires better understanding of the polymerization processes. One of the most powerful methods of synthesis of well defined polymer materials of complex architecture is Controlled Radical Polymerization (CRP) in particular Atom Transfer Radical Polymerization (ATRP). Compared with the conventional radical polymerization where initiation is slow and chain growth is very fast, the CRP processes provides better control of molecular architecture and yield gels with preserved chain-end functionality and more homogeneous structure.

In this work Monte Carlo simulations of ATRP copolymerization of monomer and divinyl cross-linker using the dynamic lattice liquid model (DLL) based on the cooperative motions concept are presented. Three cases are considered: i - random copolymerization, leading to formation of nanogels and eventually to macroscopic gelation, ii - polymerization of the monomer first and addition of the crosslinker later, leading to formation of stars via arm-first route and iii - polymerization of the crosslinker first and then addition of the monomer, leading to formation of stars via core first route. We present the structural properties of the polymers obtained for various initial crosslinker/monomer ratios in the bulk and in diluted systems. It was found, that DLL simulations allow to predict gel points in various ATRP experiments, in agreement with experimental data and the effect of solvent dilution on the gel points. Molecular weights, polydispersities and the distribution of linear chains in stars and branched copolymer molecules can be modeled as a function of input concentrations and conversion.

ACKNOWLEDGMENTS

The authors gratefully acknowledge the financial support of this research by the National Science Centre of Poland, grant UMO- 2014/14/A/ST5/00204.