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A Novel Efficient Hybrid Algorithm for Monte Carlo Simulation of Controlled Radical Polymerization: The Method Integrating Reactive and Deactivated Species

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Abstract

A hybrid stochastic-deterministic method for modeling of processes embodying fast equilibration reactions is devised. Its application to modeling controlled radical copolymerization is presented. Hundreds times shorter simulation time is achieved without sacrificing the accuracy of the results. This is documented by comparison of the new method with standard Gillespie algorithm as well as with a chain-by-chain one. The speed up effect is achieved by integrating dormant species and free radicals originating from them into one category.

Keywords: Living/Controlled Radical Copolymerization; Monte Carlo algorithm; modeling; kinetics, microstructure, chain lengths distribution

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