

Accepted Manuscript

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

Stanislaw Sosnowski, Ryszard Szymanski

PII: S1385-8947(18)31871-0
DOI: <https://doi.org/10.1016/j.cej.2018.09.154>
Reference: CEJ 19993

To appear in: *Chemical Engineering Journal*

Received Date: 9 July 2018
Revised Date: 17 September 2018
Accepted Date: 20 September 2018



Please cite this article as: S. Sosnowski, R. Szymanski, A Novel Efficient Hybrid Algorithm for Monte Carlo Simulation of Controlled Radical Polymerization: The Method Integrating Reactive and Deactivated Species, *Chemical Engineering Journal* (2018), doi: <https://doi.org/10.1016/j.cej.2018.09.154>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

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

Stanislaw Sosnowski* and Ryszard Szymanski*

Center of Molecular and Macromolecular Studies, Polish Academy of Sciences, Sienkiewicza 112, Lodz,
90-363, Poland

E-mail: stasosno@cbmm.lodz.pl, rszymans@cbmm.lodz.pl

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

Founding: This work was supported by the National Science Center, Poland, Grant No. DEC-2014/15/B/ST5/05321.

Declarations of interest: none

Download English Version:

<https://daneshyari.com/en/article/11016673>

Download Persian Version:

<https://daneshyari.com/article/11016673>

[Daneshyari.com](https://daneshyari.com)