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Author: Erlita Mastan Xiaohui Li Shiping Zhu

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Modeling and Theoretical Development in Controlled Radical Polymerization

Erlita Mastan, Xiaohui Li, Shiping Zhu*
Department of Chemical Engineering, McMaster University,
1280 Main St. West, Hamilton, Ontario, Canada L8S 4L7

Abstract

Controlled radical polymerization (CRP) systems have gained increasing interests for the past two decades. Numerous publications may be found in the literature reporting experimental and modeling work on various CRP processes, including their use in surface modification through grafting. Knowledge of underlying mechanism behind polymerization systems is valuable for product design and process optimization. This information may be obtained through the combination of modeling and experimental studies. In this review, published studies on kinetic and stochastic based modeling for CRP systems are summarized. Their relevance in model discrimination of proposed mechanisms is discussed. This review also includes various parameter estimation studies, that is crucial to obtain accurate simulation predictions. Existing issues on the fundamental mechanism in CRP processes are also addressed.

Keywords: Atom transfer radical polymerization (ATRP); Controlled radical polymerization (CRP); Modeling; Nitroxide-mediated polymerization (NMP); Reversible addition-fragmentation chain transfer (RAFT); Reversible deactivation radical polymerization (RDRP)

*Correspondence to: zhuship@mcmaster.ca; +1-905-525-9140 ext 24962