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Extended Abstract

Green Degradable (Co)Polyacrylics: A Kinetic Monte Carlo Study †

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One of the major challenges for today's society is the management and handling of plastic/polymer waste. Two main solutions have been suggested to tackle this issue: (i) recycling of the currently existing bulk polymers either through mechanical, thermal, or chemical treatments, and (ii) the development of degradable substitutes with the same (or even better) properties as those of the conventional bulk polymers. A bottleneck in both cases is represented by the limited understanding of the degradation of polymer materials on a molecular level, as polymer chains tend to break first at certain functional groups or structural defects, of which the location and prevalence are highly important. In this work, we present a unified matrix-based elementary-step-driven kinetic Monte Carlo (kMC) framework to model both the polymerization and degradation of conventional and (bio)degradable polymer materials. This kMC framework is able to track the location and quantity of these structural defects or functional groups throughout both polymerization and degradation. This model is able to track the location and quantity of these structural defects or functional groups throughout both polymerisation and degradation. The ultimate focus is on the radical copolymerization of methyl methacrylate (MMA) with 2-methylene-1,3-dioxepane (MDO) and the subsequent hydrolysis of the resulting poly(MMA-MDO) toward biodegradable and functional oligomers [1,2]. We highlight the relevance of product heterogeneity resulting from batch operation and its influence on the (bio)degradation of the copolymers.

Supplementary Materials: The following are available online at https://www.mdpi.com/2504-3900/69/1/11/s1.

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