kinetic Monte Carlo Simulations of Poly(styrene peroxide) Chemical Recycling

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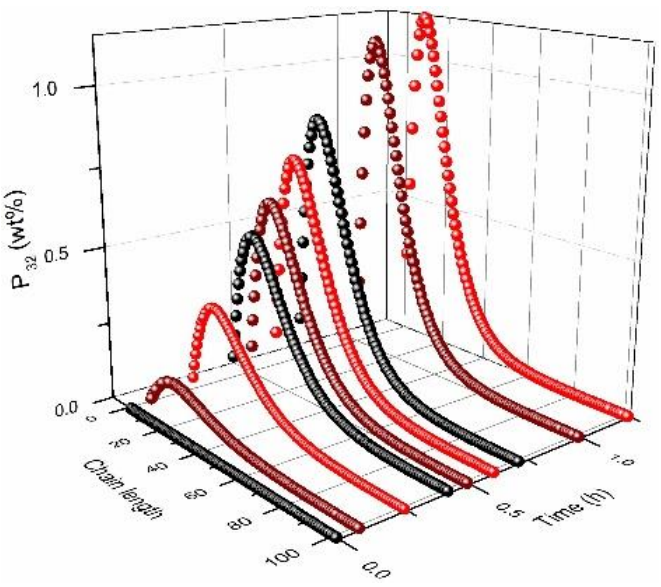
Abstract



Over recent decades, technological advances, population increase, and lifestyle changes have increased the amount of municipal solid waste (MSW) drastically, in which solid plastic waste (SPW) constitutes a significant part. Chemical recycling technologies, *e.g.* pyrolysis, will be one of the most important contributors to solve the problem of SPW disposal via upcycling within the circular economy approach. In this work, a detailed kMC model for the isothermal (100°C) pyrolysis of polydisperse PSP was developed as a proof-of-concept. All essential reactions are implemented using binary trees for fast and accurate calculation of reaction probabilities. The so-called "mass-weighted" binary trees are used for the kMC sampling of peroxide bond fissions and hydrogen abstractions. Furthermore, a kinetic parameter tuning strategy using artificial neural networks (ANNs) is used to flawlessly predict published experimental data. The generated data set was also utilized as a sensitivity analysis to unravel the effects of individual reactions on the experimental responses. The model is successfully validated against the reported evolution of the peroxide bond content and product distributions. The time-resolved 3-dimensional mass-fraction (wt%) molar mass distributions (MMDs) of a polymer side-product P_{32} during the entire course of degradation is presented in the **Figure**. The nature of the competing unzipping reactions during the degradation process and the two-stage degradation behavior is analyzed using both instantaneous and time-averaged concentrations. The essentiality of the implemented mass-weighted trees is proven by analyzing the hydrogen abstraction reaction frequencies. Novel investigation techniques presented in this work will aid as a proof-of-concept for detailed analyses via kMC in future polymer degradation studies that are significant for chemical recycling processes. Creating detailed kinetic models for polymers abundant in SPW, *e.g.*

polyethylene (PE) and polystyrene (PS), will aid in boosting the chemical recycling potential of these polymers by assisting in the design and optimization of innovative reactor technologies.

Keywords:

Chemical Reaction Engineering

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