PUSHING FORWARD THE PREDICTIVE POWER OF KINETIC MONTE CARLO SIMULATIONS FOR DETAILED (DE)POLYMERIZATION CHEMISTRIES

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Polymers consist of molecules with a broad spectrum of chain lenghts, branching levels and compositions. A classical characterization of polymers is devoted to averages, or in case distributed molecular properties are aimed at, the interpretation is often limited to one or two variables and the measurement is relative.

Recent advances in the field of polymer reaction engineering [1-3] have enabled to track the detailed make-up of individual molecules up to the industrial scale *via* additional compartment coupling, with model validation of chemical and diffusional parameters *via* independent techniques.

The current contribution highlights the strength of coupled matrix-based kinetic Monte Carlo (CMMC) simulations to advance the field of macromolecular engineering and design. Case studies include ionic and (controlled) radical polymerization routes, addressing a variety of topology levels transcending from linear to fully crosslinked systems [4,5]. Attention is also given to degradation reactions and recycling goals [6], highlighting the general potential of stochastic modeling frameworks.

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