Kinetic Monte Carlo Simulations of Flow-Assisted Polymerization

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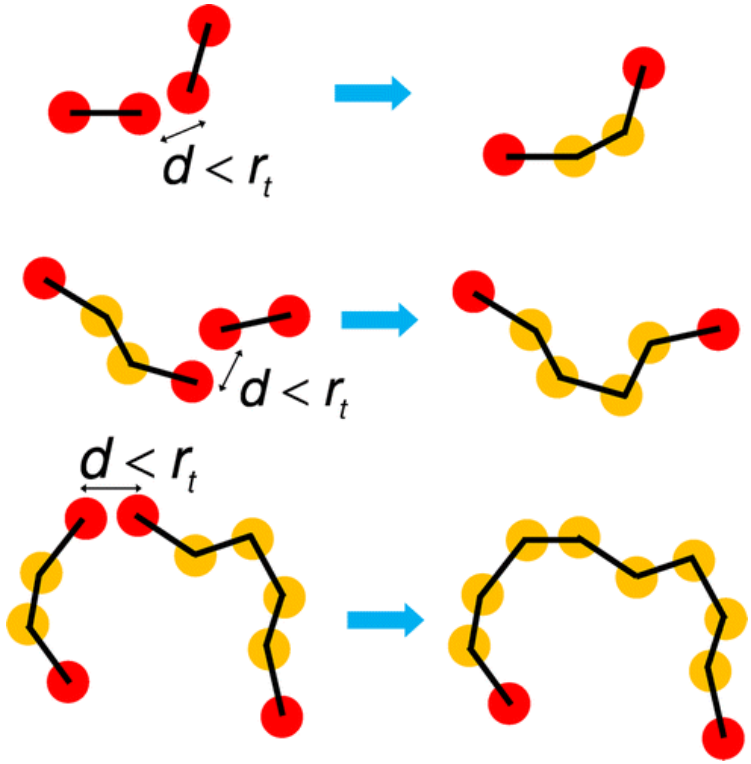
We performed kinetic Monte Carlo simulations on a model of a polymerization process in the presence of a periodic oscillatory flow to explore the role of mixing in polymerization reactors. Application of an oscillatory flow field helps overcome the diffusive limitations that develop during a polymerization process due to an increase in the molecular weights of polymer chains, thereby giving rise to high rates of polymerization. A systematic increase in the flow strength results in a “dynamic” coil–stretch transition, leading to an elongation of polymer chains. Reactive ends of stretched (polymer) chains react more frequently than the reactive ends of coiled chains, which are screened by other monomers of the same chain. There exists a critical flow strength for the efficiency of polymerization processes. The kinetic Monte Carlo simulation scheme developed here exhibit great promise for the study of dynamic properties of polymer systems.

The methods developed in this communication can be applied to the study of polymer systems under influence of more complex flow fields or other kinds of external fields (e.g., electric field, magnetic fields, etc.).



We model a system of dimers with reactive ends (red) that combine to form longer chains having inert intermediate beads (yellow) when they come close within a threshold distance r_t.

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