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Monte Carlo study of confinement effects on controlled radical polymerization reactions SALOMON TURGMAN-COHEN, JAN GENZER, North Carolina State University — Bulk- and surface-initiated controlled radical polymerization (CRP) in implicit solvents is modeled using a stochastic Monte Carlo algorithm by implementing the bond-fluctuation model scheme. We study the effect of system parameters, including: bulk vs. surface initiation, surface density of initiators, substrate geometry, solvent quality, and the ratio between surface and bulk polymers on the molecular weight and polydispersity index (PDI) of the resulting polymers. To better understand the effect of geometry and steric hindrance on the polymerization we calculate the sizes and shapes of the growing polymers and monitor the various reactive species located near the reactive polymer chain-ends. Our results indicate that confinement of the growing chains has detrimental consequences on the ability of CRP to yield nearly monodisperse polymers; i.e., confining polymers to impenetrable surfaces and/or decreasing solvent quality decreases the rate of polymerization and increases the PDI.

Salomon Turgman-Cohen
North Carolina State University

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