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Computer simulation study of solvent quality and reaction geometry on controlled radical polymerization SALOMON TURGMAN, JAN GENZER, North Carolina State University — Bulk- and surface-initiated controlled radical polymerizations are simulated using a stochastic Monte Carlo algorithm by following the bond-fluctuation model scheme and an attractive potential acting among bonded monomer beads. Specifically, we investigated the changes in polymer molecular weight and molecular weight polydispersity index (PDI) due to conformational variations of the chains that occur upon altering solvent quality. Variations in reaction geometry, temperature, initial monomer and initiator concentration, probability of initiation, initial probability of monomer addition, probability of termination, fraction of living polymers and their lifetime were studied. Synergistic effects among these parameters and the geometry of the reaction were also explored. Preliminary results suggest that polymerization in poor solvent quality solvents result in shorter polymers and increased molecular weight PDI.

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