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Kinetics of loop formation in worm-like chain polymers REZA AFRA, BRIAN TODD, Purdue University — Polymer cyclization occurs during polymerization reactions as well as in many biological processes involving biopolymers. A common theoretical approach to calculating cyclization reaction kinetics is to approximate a high-dimensional conformational search with a one-dimensional diffusion along an effective reaction coordinate. We employed Brownian dynamics simulations to test the validity of this approximation for cyclization kinetics in the worm-like chain polymer model. This model is often used to describe polymers that exhibit backbone stiffness beyond the monomer length scale. We find that one-dimensional diffusion models overestimate the mean cyclization time and do not predict the quantitatively correct dependence of cyclization time on chain length or capture radius. Our findings highlight the difficulty of describing high-dimensional polymers with simple kinetic theories.

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