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(G*) The Limits of Polymer Single File Dynamics: A phase diagram

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We use Langevin dynamics (LD) simulations to investigate single file diffusion (SFD) in a dilute solution of flexible linear polymers inside a narrow tube. The transition from single-file diffusion, where the mean-square displacement scales like $\langle x^2 \rangle \sim t^{1/2}$, to normal diffusion with $\langle x^2 \rangle \sim t$, is studied as a function of the system parameters, such as the width of the channel, the polymer concentration and the polymer size. Based on our simulation results and scaling arguments, we propose a phase diagram describing the different diffusion regimes. We also map this problem onto a one-dimensional Lattice Random Walk algorithm where the diffusing object represents the polymer's center of mass. In order to model the polymers entanglement and disentanglement processes we allow several objects to temporarily share the same lattice site and diffuse together. Extension of our work to polydisperse polymer solutions, one-dimensional electrophoresis, ring polymers and DNA mapping are discussed.

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