

Transport dynamics of comb-like polymers in confined environments driven by external forces: A simulation study

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Abstract

We examine the translocation dynamics of comb-like polymers through confined environments under an externally applied force using computational simulations. Two distinct simulation approaches and systems are employed: (1) Monte Carlo (MC) simulations to study polymer translocation through a simplified pore under an imposed electric field, and (2) Langevin dynamics (LD) simulations to investigate polymer transport through a nanochannel subjected to a pulling force applied on a terminal monomer of the backbone. The study systematically explores a broad range of system parameters, including chain size, backbone length, side-chain length, grafting density, and applied force/field magnitude. For electric field-driven translocation, the mean translocation time exhibits a non-monotonic dependence on the field strength, with a critical threshold marking the transition between smooth and chaotic translocation regimes. In the case of nanochannel confinement under a pulling force, the mean exit time similarly displays a non-monotonic relationship with grafting density, peaking at an optimal grafting density that maximizes translocation time. In both scenarios, the mean translocation time scales linearly with backbone and side-chain lengths.