

Abstract Submitted
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Dissipative particle dynamics simulations of dilute polymer solutions confined in a slit with interactive surfaces WENHUA JIANG, Department of Chemistry, The University of Memphis, Memphis, TN 38152 , JIANHUA HUANG, Department of Chemistry, The University of Memphis, Memphis, TN 38152; Department of Chemistry, Zhejiang Sci-Tech University, Hangzhou, 310018, China, MOHAMED LARADJI, Department of Physics, The University of Memphis, Memphis, TN 38152, YONGMEI WANG, Department of Chemistry, The University of Memphis, Memphis, TN 38152 — Dynamics of polymer chains in confined geometries are significantly different from that in a bulk solution. Understanding the confinement effect on the chain dynamics is of great value to applications of microfluidic devices. We applied dissipative particle dynamics (DPD) to study polymer chain dynamics confined in slits with interactive surfaces. We first examined the dynamics and the static properties of polymers in dilute bulk solutions. After correcting for the effect of finite box size, our results unambiguously confirmed that the DPD has correctly accounted for hydrodynamic interaction within a polymer chain. We then extended the simulation to polymer solutions confined in a slit with interactive surfaces. For purely repulsive surfaces, the dynamics and the static properties of polymers show a broad crossover from a free solution to a confined solution. The attractive interactions of polymers with the walls were found to retard the dynamics of the chains significantly. The influence of surface interactions on polymer dynamics will be presented.

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