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Multiple Particle Collision Dynamics Simulations of the Effect of Catenation on the Structural and Dynamic Properties of Ring Polymers in Solution GOVIND HEGDE, RAJESH KHARE, Department of Chemical Engineering, Texas Tech University — Multiple particle collision dynamics (MPCD) is a particle based mesoscale simulation technique that coarse-grains the solvent while preserving the hydrodynamics, thus enabling simulations over longer length and time scales as compared to molecular dynamics (MD) simulations. In this work, MPCD is used to study the effect of topology on the structural and dynamic behavior of complex fluids. The systems of interest in this work are the dilute solutions of ring and catenated ring polymers. MPCD simulation results are compared with those obtained from MD simulations in which the hydrodynamic interactions are governed by the explicit intermolecular interactions. Different chain topologies are considered such as catenated as well as multi-catenated rings. Results will be presented for the effect of chain length on the radius of gyration and chain diffusion coefficient for the various topologies studied. Our results will also be compared with previous theoretical and experimental work reported in literature.

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