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Behavior of a nano-particle and a polymer molecule in a nano-scale four-roll mill MINH VO, DIMITRIOS PAPAVASSILIOU, The University of Oklahoma — The four-roll mill device could be used to create a mixed flow from purely extensional stresses to completely rotational through the proper selection of speed and direction of each of the four cylindrical rollers. Considerable research has been done with this device for macroscale rheological studies.. In our study, the dissipative particle dynamics (DPD) method was employed to investigate the behavior of a nano-sphere and a polymer molecule in different conditions within a four-roll mill device. Hydrophilic properties of each roll were generated by adjusting interaction parameters and using bounce back boundary condition at the solid surface. All simulations were run up to 4×10^6 time steps at room temperature using the open source LAMMPS package. After the flow in the system reached equilibrium, a nano-sphere and then a polymer chain were released at the center of the simulation box. Their trajectories were recorded at different shear rate conditions. The propagation of nanosphere in different rotational flow will be discussed. Additionally, the deformation of polymer chains will be compared to that in a simple shear flow.

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