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Mesoscale simulation of entangled polymers: Part II. Lowe-Andersen thermostat SHAGHAYEGH KHANI, MIKIO YAMANOI, JOAO MAIA, Case Western Reserve University — Dissipative Particle Dynamics (DPD), despite its good potential in simulating soft matter, has some limitations when studying the entangled polymer systems. First limitation which arises from utilizing soft potentials in DPD is associated with unphysical bond crossings. The bond crossings can be avoided by introducing a segmental repulsive potential to the bonds. Another deficiency of DPD in simulating fluids is related to the Schmidt number. In standard DPD the momentum and mass transfer at the same rate and thus this dimensionless number takes a gas-like value (~ 1) when simulating fluids. In order to overcome this problem a Lowe-Andersen thermostat was used as an alternative method to DPD and the thermostat was found to be more successful in controlling the temperature in equilibrium state (independent from the time step) and over a wide range of shear rates. The ability of the method in capturing the entanglement effect and reproducing the static and dynamic properties of polymer melts and the scaling laws were investigated and the results were compared to the ones from standard DPD. The performance of the method in capturing the main features of the shear flow and reproducing linear and nonlinear viscoelastic properties was also evaluated.

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