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Mesoscale simulation of the rheology of high molecular weight polymer gels YELENA SLIOZBERG, JOHN BRENNAN, TIMOTHY SIRK, JAN ANDZELM, U. S. Army Research Laboratory — Polymer gels are comprised of physically or chemically cross-linked polymers that are highly swollen with solvent. The rheology of these gels depends on their morphological properties, such as the number of bridging chains and trapped entanglements. The prediction of structural and mechanical properties of gels using computational approaches is challenging and requires advanced particle-based mesoscale methodologies. Recently, we have implemented an approach to predict mechanical properties of high molecular weight block copolymers by allowing for chain entanglement behavior within the dissipative particle dynamics (DPD) methodology. Diffusion coefficients have been evaluated to locate the crossover from the Rouse to reptation dynamics. In this talk, we will demonstrate that including a segmental repulsive potential in addition to the usual DPD framework can prevent chain crossings and leads to an improved representation of mechanical and structural properties of polymer gels.

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