Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Entanglement effect in polymer melts by Dissipative Particle Dynamics (DPD) SHAGHAYEGH KHANI, JOAO MAIA, Case Western Reserve University — Dissipative Particle Dynamics (DPD) is a mesoscale simulation method that has shown a very good potential in modeling different soft matter systems from colloidal suspensions to highly entangled polymers. Like any other simulation technique DPD is associated with some deficiencies, for instance in the case of entangled polymers soft repulsions used in DPD allow particle overlap which may result in topology violations that prevent the correct capturing of the entanglement effect. Therefore, in the present work in order to properly reproduce the dynamics and viscoelastic properties of polymers the soft repulsions between the particles are substituted with a repulsive potential between non-adjacent bonds of different FENE chains. Also, DPD is a coarse-grained simulation method that can be used to model time and length scales longer than atomistic models; however, due to the existence of an upper level limit for the level of coarse graining this method is not applicable for the whole mesoscopic range. Thus, this work represents a new approach for tuning the level of coarse-graining by adjusting the simulation parameters. The ability of the method in capturing the entanglement effects is validated by simulating dynamic and viscoelastic properties of polymers.

Shaghayegh Khani
Case Western Reserve University

Date submitted: 16 Nov 2014 Electronic form version 1.4