Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Coarse-grain Tunable Dissipative Particle Dynamics: Droplet Dynamics in Micro- and Nano-emulsions ARMAN BOROMAND, JOAO MAIA, Case Western Reserve University — Due to the multiscale phenomena in droplet dynamics from single droplets to highly concentrated emulsions (HCE) on one hand and complexity of the problem on the other hand, there is a need for a mesoscale simulation technique to capture the right underlying physics in these systems. This makes Dissipative Particle Dynamics (DPD) a suitable candidate, since it is capable of capturing microscopic phenomena and provide comparison to macroscopic simulations and experiments, within a reasonable calculation time compared to Molecular Dynamics (MD). In this presentation, we focus on the interplay between droplet size and the stress level in shear flows for three different combinations: Newtonian/non-Newtonian droplet in Newtonian/non-Newtonian matrix. The geometrical changes in these three cases will be compared to macroscopic models and experimental results and the validity of this mesoscopic simulation will be discussed. In addition, the dependency of surface tension to droplet size in the case of Newtonian droplets in Newtonian matrix is shown and the effect of this term on the dynamics of nanoscopic droplets is discussed. For the case of non-Newtonian droplets, their dynamics is studied for polymer chains with different molecular weight and chain characteristics.

Arman
Case Western Reserve University

Date submitted: 15 Nov 2013 Electronic form version 1.4