Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Coarse-graining of Polystyrene in Various Environments by Iterative Boltzmann Inversion[1] ROLAND FALLER, BESTE BAYRAMOGLU, UC Davis, Chemical Engineering & Materials Science — We have developed mesoscale models for polystyrene (PS) oligomers in various environments following the Iterative Boltzmann Inversion Technique for polymer coarse–graining with and without confinement. Bond, bending angle, torsion angle distributions and radial distribution functions between PS monomers show that local structures were reproduced very well, while a small discrepancy remained in the reproduction of global structures (radii of gyration and end–to–end distances), which is probably due to end effects. Speed–up in polymer dynamics with each model was monitored by scaling factors calculated based on characteristic relaxation times of the end monomers as well as diffusivities of the chains. Results show that coarse–graining is most successful for the highest concentration system (melt) and least for the lowest concentration (dilute solution) due to the stronger slowdown of diffusive and rotational dynamics in atomistic simulations with concentration. The speed–up in the confined solution system was found to be greater than in the unconfined solution system due to the same reason except that confinement slows down the dynamics in that situation. We also characterize the limits to which extent the same models can be used for different degrees of confinement.

[1]Supported by U.S. Department of Energy, Office of Science, Basic Energy Sciences (grant number DE-FG02-06ER46340).

Roland Faller
UC Davis, Chemical Engineering & Materials Science

Date submitted: 31 Oct 2012 Electronic form version 1.4