Abstract Submitted
for the DFD10 Meeting of
The American Physical Society

Examining the coil-stretch transition in flexible polymers
PATRICK UNDERHILL, RANGARAJAN RADHAKRISHNAN, Rensselaer Polytechnic Institute — The behavior of polymer solutions in elongational flow is important in many applications. An especially important property is the dramatic strain rate hardening resulting from the coil-stretch transition. Predictions of the coil-stretch transition and hysteresis have been verified by visualizing single molecules of double-stranded DNA (ds-DNA). The same behavior has not yet been directly observed in single molecule studies of synthetic polymers or more flexible biopolymers such as single-stranded DNA. Current theories of flexible polymers predict these other polymers will behave in a similar way to ds- DNA. However, we have very recently predicted that these other polymers could have dramatically different behavior; the coil- stretch transition can be eliminated under some conditions. For this purpose, we have altered the common bead-spring chain polymer models and simulated their response in flow using Brownian dynamics (BD). This new model we developed allows us to capture the importance of flexibility, entropic elasticity, hydrodynamic interactions, and solvent quality in an accurate and efficient way. This would have not been possible using conventional methods of including excluded volume as a repulsive interaction potential between beads; such a model would require such a large number of beads interacting that it would not be computational tractable.

Patrick Underhill
Rensselaer Polytechnic Institute

Date submitted: 06 Aug 2010 Electronic form version 1.4