Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Cyclization of Rouse Chains at Long and Short Time Scales[1]
CHUCK YEUNG, Pennsylvania State University at Erie, The Behrend College, BARRY FRIEDMAN, Sam Houston State University — We have investigated cyclization of a Rouse chain at long and short times by a Langevin dynamics simulation method. We measure $S(t)$, the fraction of non-reacted chains, for chains lengths ranging from $Z = 5$ to $Z = 800$. Comparison is made with the closure approximations of Wilemski and Fixman and Doi and the renormalization group (RG) arguments of Friedman and O'Shaughnessy. The ratio of the long time reaction time scale to the Rouse time, $T = \tau/\tau_R$ is predicted to approach a constant value for long chains independent of the reaction capture range. However, the two theoretical approaches predict different values for T^* the long chain limit of T. Our simulations find that $T^* \approx 1.75$ much closer to the RG prediction of $\pi^3/16 = 1.94$ than the Wilemski-Fixman-Doi prediction of $T^* = 2.17$. More convincing evidence for the RG analysis is obtained by comparing the short time decay of $S(t)$ to long time results. The RG analysis predicts that $S(t)$ should decay as a power law at early times and that the exponent in the power law α is related to T by simple expression with no free parameters. Our simulations find remarkable agreement with this parameter free prediction even for relatively short chains.

[1]Partially supported by NSF DMR-9986879

Chuck Yeung
Penn State Univ at Erie, The Behrend College

Date submitted: 30 Nov 2004 Electronic form version 1.4