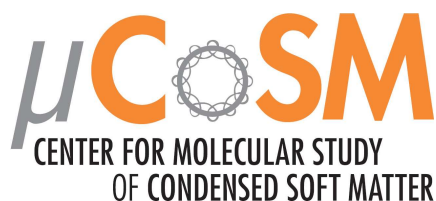


Jay D. Schieber
Department of Chemical and Biological Engineering, and Director:
Center for molecular study of condensed soft matter (μ CoSM)
Illinois Institute of Technology



Multiscale modeling of macromolecular dynamics in entangled environments

At very small mass fractions, polymers extend sufficiently in solvent to begin interacting with one another. At yet higher concentrations, they become entangled with one another, and these entanglements are generally believed to dominate their dynamics, even for very lightly entangled chains. We will show how thermodynamic and statistical mechanical analysis of experimental data essentially prove the existence of entanglements. Then, a simple coarse-grained mathematical model is presented that predicts quantitatively nearly all experimental data studied on the rheology of concentrated linear polymer liquids—solutions or melts. The model is applicable to linear, branched or cross-linked chains, and even DNA electrophoresis in gels or polymer solutions. These predictions are made with only two phenomenological parameters: β to describe the entanglement density, and τ_K to describe the time scale of the smallest smallest statistical element (a Kuhn step) in the chain. Recent atomistic simulations [1–3] have shown an ability to predict the first parameter β by studying the topology of concentrated polymers at equilibrium. More detailed statistics from these simulations also agreed with the proposed mathematical model [4].

References

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