MAR15-2014-001867

Abstract for an Invited Paper
for the MAR15 Meeting of
the American Physical Society

From molecules to non-linear rheology of highly branched, entangled polymers: getting your priorities right

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The tube model for polymer dynamics offers the promise of predicting the flow properties of entangled polymeric liquids. Given a knowledge of the sizes and shapes of the polymers, the tube model suggests dynamical rules for the relaxation of stress carried by the molecules. Over the last couple of decades these rules have been, for the most part, established through experiments and simulations on liquids containing molecules of well-defined size and shape. For prediction of small amplitude flows, these rules are now codified in computer algorithms such as Larson's hierarchical model (http://www.engin.umich.edu/dept/che/research/larson/) and our own "BoB" model (http://sourceforge.net/projects/bob-rheology). As a result, it is now possible to make meaningful predictions for flow properties of industrial polymeric resins with distributions of randomly branched structures. Since real polymers are subjected to large deformations in realistic processing, we have recently extended the above work to prediction of the large-deformation response of branched polymers. This talk will describe the extra physics that applies in the non-linear flow regime, and how this has been implemented in our model: the central message is that one needs to know three quantities for every strand in the resin: 1) an orientation relaxation time, (2) a stretch relaxation time, and (3) a limiting value for the chain stretch. The latter is often discussed in terms of a topological quantity known as "priority." Motivated by recent experiments on well defined "comb" molecules, we discuss some shortcomings in our current prediction of the "priority" and how this may be improved upon.