Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Predicting non-linear rheology of randomly branched entangled polymer melts[1] DANIEL READ, CHINMAY DAS, MICHAEL KAPNISTOS, University of Leeds, TOM MCLEISH, University of Durham — We recently published a computational algorithm [C. Das et al Journal of Rheology 50, 207-235 (2006)] for predicting the linear rheology of arbitrarily branched polymer melts, which was successfully used for well defined architectures (stars, combs, Cayley trees etc.) and well-characterised industrial resins. We now discuss an extension to the non-linear regime, via a mapping onto a multi-mode "pom-pom" ensemble. There is, in principle, sufficient information in the algorithm to do this without additional free parameters. However, the procedure is not exact and one must consider the most important physics to represent. In particular, we highlight the need to distinguish between stress relaxation via constraint release and via tube escape. We also discuss the topological "priority" variable (which limits the stress in extension) and the considerations needed when assigning this to each polymer strand (which polymer segments should one count as relaxed?) In doing this, and as a result of tube advection, we find we need to introduce a new variable ("altitude") related to the topological distance of a strand from the molecule centre.

[1]EPSRC - Microscale Polymer Processing 2 grant

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Date submitted: 18 Nov 2009 Electronic form version 1.4