Comparing tube models for predicting the linear rheology of branched polymer melts ZUOWEI WANG, XUE CHEN, RONALD LARSON, University of Michigan, Department of Chemical Engineering — The hierarchical [1,2] and bob (or branch-on-branch) [3] models are tube-based computational models developed for predicting the linear rheology of general mixtures of polydisperse branched polymers. These two models are based on a similar tube-theory framework, but differ in their numerical implementation and details of relaxation mechanisms. We present a detailed overview of the similarities and differences of these models, and examine the effects of these differences on the predictions of the linear viscoelastic properties of a set of representative branched polymer samples, in order to give a general picture of the performance of these models. Our analysis confirms that the hierarchical and bob models quantitatively predict the linear rheology of a wide range of branched polymer melts, but also indicate that there is still no unique solution to cover all types of branched polymers without case-by-case adjustment of parameters such as the dilution exponent $\alpha$ and the factor $p^2$ which defines the hopping distance of a branch point relative to the tube diameter. An updated version of the hierarchical model, which shows improved computational efficiency and refined relaxation mechanisms, is introduced and used in these analyses. [1] R. G. Larson, Macromolecules 34, 4556 (2001). [2] S. J. Park et al., Rheol. Acta 44, 319 (2005). [3] C. Das et al., J. Rheol. 50, 207 (2006).

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