

## Non-Equilibrium Molecular Dynamics Simulation of Dendrimers under Shear

L. Lue<sup>C, S</sup>

*Department of Chemical Engineering, UMIST, Manchester, United Kingdom*

J.T. Bosko, B.D. Todd and R.J. Sadus

*Centre for Molecular Simulation, Swinburne University of Technology, Hawthorn, Victoria, Australia*

Dendrimers are a relatively new class of highly branched polymers consisting of short chain units with multifunctional groups at both ends. Starting from an initiator core, the successive reaction of the functional groups with other units generates a highly branched molecule which resembles a Cayley tree [1,2]. Theoretical work on dendrimers has focused largely on determining the structure of isolated homogeneous dendrimers. Numerical self-consistent mean-field calculations have also been performed for individual dendrimers. Some molecular simulation studies have been reported to determine the structure of isolated [3] and bulk [4] homogeneous dendritic polymers; however, the focus of these simulation studies has been exclusively equilibrium properties.

The unique nature of dendrimers means that significant differences could be reasonably expected in their transport properties compared with other polymers of similar size. In this work, we use non-equilibrium molecular dynamics (NEMD) [5,6] to investigate the behavior of dendrimers under shear. The shear viscosity, energy and pressure are reported for generation up to 4 using both constrained bonds and FENE bonds. NEMD results are also presented for linear polymers of similar molecular weight. The results indicate dendrimers behave differently with respect to the onset of non-Newtonian behavior compared with linear polymers.

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