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Effect of Chain Architecture on the Structural and Rheological Properties of Dilute Polymer Solutions: A Molecular Simulation Study FARDIN KHABAZ, RAJESH KHARE, Department of Chemical Engineering, Texas Tech University — Advances in chemistry have allowed synthesis of polymer chains of specified architecture. The effect of chain architecture on the structure and rheology of dilute polymer solutions is not fully understood. Furthermore, possible breakage of polymer chains at high shear rates is important for several industrial applications. In this work, these effects are investigated by performing molecular dynamics simulations. Structure and rheology of dilute polymer solutions containing four types of chains - linear, comb shaped, H-shaped and star - are compared. Simulations are used to determine the scaling of the intrinsic viscosity with molecular weight for chains of different architectures. These simulation results are also compared with theoretical predictions from literature. In addition, structural stability of the chains is studied by monitoring their local deformation at high shear rates. Possible sites for chain scission are identified from these high shear rate simulations for each type of chain architecture.

> Fardin Khabaz Department of Chemical Engineering, Texas Tech University

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