

Abstract Submitted  
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***A priori* Determination of the Rheological Properties and Slip Phenomena of Polymer Melts**<sup>1</sup> JOHN DORGAN, NICHOLAS RORRER, Colorado School of Mines, CHEMICAL AND BIOLOGICAL ENGINEERING TEAM — This work builds on previous studies...<sup>1,2</sup> done utilizing a coarse grained Dynamic Monte Carlo algorithm. The algorithm is able to capture the molecular scale details of flowing polymer melts in nanoscopic geometries. In shear flow all of the known observable viscoelastic behavior associated with polymer melts is predicted in a completely *a priori* manner. For example, the correct scaling of the zero shear viscosity with molecular weight is observed. When polydispersity is introduced, the viscosity curves demonstrate a broadening behavior, exhibiting the same zero shear viscosity but lower viscosities at higher shear rates. Slip phenomena has been investigated under both shear (Couette) and parabolic (Poiseuille) flow. These two different flow cases are demonstrated to be profoundly different in their molecular scale details. All of the predicted results are in *post facto* agreement with many experiments and help shed fundamental insight into the molecular scale behavior of polymer fluid dynamics. .1. Dorgan, J. R.; Rorrer, N. A.; Maupin, C. M., *Macromolecules* **2012**, *45* (21), 8833-8840. 2. Dorgan, J. R.; Rorrer, N. A., *Physical Review Letters* **2013**, *110* (17)

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