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Rheological properties of polymer melts in confined shear flow from dynamic Monte Carlo simulations. JOHN DORGAN, Colorado School of Mines — The viscoelastic properties of dense polymer melts in shear flow are examined using dynamic Monte Carlo simulation for plate spacings less than 10 times the molecular radius of gyration. The coarse graining methodology employed consists of the cooperative motion algorithm of Pakula and a derived biasing technique based on previous studies of Binder and Baushnagel. For relatively large plate spacings and slow flows, a uniform linear velocity profile is obtainable. Use of the Kramers form for entropic springs allows the calculation of stress in the simulation providing a means for exploring rheological properties including viscosity and normal stress differences. Results are in excellent agreement with well-established experimental facts; a shear thinning viscosity is obtained, the first normal stress difference increases with shear rate, and the first normal stress coefficient decreases with shear rate. Evidence of entanglements are present for longer chain lengths. For fast flows, the linear velocity profile is lost and shear banding is observed. A non-monotonic stress with shear rate is found in conjunction with the shear banding and mechanistically this is attributable to a cohesive failure with an excess of chain ends being found at the slip plane. Results for variable plate spacings shed some insight into novel confinement effects that are being exploited in emerging areas of nanotechnology.

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