Abstract Submitted
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Scaling of viscosity with rate, pressure, and temperature: Linking simulations to experiments[1] VIKRAM JADHAO, MARK ROBBINS, The Johns Hopkins University — Elastohydrodynamic lubrication (EHL) is important in many practical devices and produces extreme pressures (> 1 GPa) and shear rates ($10^5 - 10^7$ s^{-1}). This makes EHL fluids ideal candidates for bridging the gap between experimental and simulation studies of viscosity. There is an ongoing debate about whether the high-rate response of simple molecules like squalane follows a power-law Carreau model or a thermal activation based Eyring model. We use molecular dynamics simulations to investigate the rheological response of squalane for a wide range of rates ($10^5 - 10^{10}$ s^{-1}), pressures (0.1 MPa to 3 GPa), and temperatures ($100 - 313$ K). We find that experimental and theoretical results can be collapsed onto a master curve consistent with Eyring theory over more than 20 orders of magnitude in rate. Extrapolating Eyring fits to simulations at 10^7 s^{-1} and above yields Newtonian viscosities η_0 that are consistent with available low-rate experiments, and allows predictions to much higher pressures and lower temperatures. There is no indication of a diverging viscosity at finite stress, since $\log \eta_0$ rises sublinearly with pressure up to 6 GPa and $\eta_0 > 10^{12}$ Pa-s. Correlations between chain conformations and Eyring parameters are also presented.

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