Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Predicting Viscosity of Complex Lubricant Molecules with Ester Functional Groups using Nonequilibrium Molecular Dynamics Simulations.[1] M A SABUJ, Dave C. Swalm School of Chemical Engineering, Mississippi State University., NEERAJ RAI, Dave C. Swalm School of Chemical Engineering, Mississippi State University and Center for Advanced Vehicular Systems, Mississippi State University — The knowledge of transport properties (viscosity and diffusion) are important for a number of wide range of industrial applications. Although molecular simulations have made tremendous progress in the last decade in predicting thermodynamic and transport properties based only on molecular structure, predicting viscosities with good accuracy has remained a significant challenge. Here, we use nonequilibrium molecular dynamics simulation (NEMD) to predict shear viscosity of four different but structurally similar pentaerythritol ester (PE) molecules at five different temperatures and five different pressures using the TraPPE-UA force field. Our calculations shows that TraPPE force field can predict shear viscosity values within 10 \% of experimental measurements. Furthermore, PE molecules absorb moistures from atmosphere; therefore, the change of viscosity was calculated in the presence of 5, 10 and 25 mole \% of water. Structural analysis was provided to get molecular insights and relative order of viscosity. The free volume concept can predict the pressure dependence of viscosity very well, a quantitative and rigorous analysis of the pressure dependence of viscosity was provided in terms of the free volume of the liquid.

[1]Effort sponsored by the Engineering Research & Development Center under Cooperative Agreement number W912HZ-15-2-0004.

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Date submitted: 16 Nov 2016 Electronic form version 1.4