Simulating lubricants' shear thinning considering additives – WTC 2022, Lyon

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While the search for the origins of shear thinning is ongoing, it is important to know the behavior of a lubricant during shear thinning for mechanical applications. Molecular dynamics simulations are a powerful tool to determine the lubricants' viscosities up to extreme shear rates in various settings leading to shear thinning curves for each setup. This study presents a comparison of the shear thinning of PAO4 under a variation of pressures and investigates the impact of ZnDTP molecules added to the systems as lubricants' additive.

Keywords: rheology, viscosity, shear thinning, lubricants, additives

1. Introduction

Additives are mixed into lubricants to obtain certain properties such as improved wear performance or endurance under severe pressures. To predict a lubricant's behavior in mechanical applications and to facilitate its choice, knowledge of its characteristics is needed as for instance the friction. Molecular dynamics (MD) simulations help obtaining these properties. During this study the lubricant's viscosities were evaluated under various pressures and depending on high shear rates. These very high velocities applied in shearing can be considered as extreme conditions leading to shear thinning profiles where the viscosities stop being Newtonian and decrease rapidly with higher shear rates. This study aims at the impact of additives mixed with the lubricant on the shear thinning curves.

2. Methods

2.1. Basic equation

The origins of shear thinning are subject of ongoing research. For lubricants, this effect is well fitted by the Carreau equation

$$\frac{\eta}{\eta_N} = \left[1 + \left(\frac{\dot{\gamma}}{\dot{\gamma}_0}\right)^2\right]^{(n-1)/2} \quad (1)$$

where η_N is the Newtonian viscosity, $\dot{\gamma}$ the shear rate and $\dot{\gamma}_0$ the critical shear rate quantifying the drop into shear thinning regime [1]. Using

$$\sigma = \eta \cdot \dot{\gamma} \quad (2)$$

the viscosity η can be obtained with the shear stress σ.

2.2. Simulations

The shear thinning behavior of PAO4 as lubricant is the base of this analysis. A liquid bulk containing 75 mass percent C_{30} and 25 mass percent C_{40} molecules are sheared with velocities between 10^{-2} and 800 m s^{-1} and compared for pressures of 30 MPa, 250 MPa and 500 MPa. All systems are set up with a temperature of 373 K and simulated through an all-atoms approach. Additionally, the obtained shear thinning curves are compared to other simulations where in one case 1 and in the other 10 ZnDTP molecules are mixed to PAO4.

2.3. Results

The comparison of shear thinning curves of PAO4 for three different pressures are displayed in Figure 1. The comparison of systems containing 0, 0.5 or 5 mass percent ZnDTP molecules is shown in Figure 2. The Newtonian viscosity η_N behaves as expected: it is higher for higher pressures for the same temperature [2].

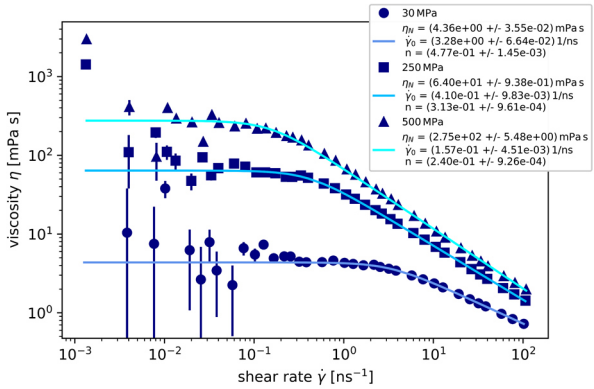

Figure 1: Comparison of shear thinning curves of PAO4 at 30 MPa (circles), 250 MPa (squares) and 500 MPa (triangles) with fits of the Carreau equation (blue lines).

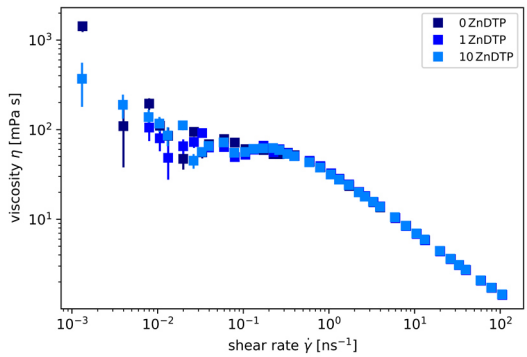

Figure 2: Comparison of shear thinning curves of PAO4 with 0, 0.5 or 5 mass percent ZnDTP as additives in systems with a pressure of 250 MPa.

3. Discussion

Furthermore, a tendency can be found: the shear thinning begins at lower shear rates for higher pressures. Moreover, the higher the Newtonian viscosity the higher seems to be the gradient of the shear thinning.
The different mixtures with the additive scarcely impact the course of the shear thinning.

4. Reference

[1] Jadhao, V. et Robbins, M. O., 2019, arXiv, 1903.03996
[2] Jadhao, V. et Robbins, M. O., PNAS July 25, 2017 114 (30) 7952-7957