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Calculation of EHL Traction for a Model Hydrocarbon Using Molecular Simulation and Rheometry

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Abstract

Recently, remarkable agreement has been reported between nonequilibrium molecular dynamics simulation and high-pressure Couette rheometry on squalane. We utilized the parameters obtained from this unique collaboration along with high-pressure viscometer measurements to calculate the elastohydrodynamic traction curve. A comparison with measured traction at 1.29 GPa shows excellent agreement, confirming the validity of the measurements and simulations. It should no longer be necessary to invoke a different rheological response to explain film thickness and traction.

Calculations

We have measured the traction of squalane at 40°C in elliptical contact using a skewed roller traction rig with a contact aspect ratio of 1.61. These data are plotted as points in the figure. The limiting low shear viscosity, μ, has been obtained[1] to a pressure of 1.06 GPa with a falling-body viscometer. Also, the constitutive behavior of squalane has been thoroughly characterized by NEMD and high-pressure Couette rheometry resulting in published[2] values of the Carreau parameters and a validation of standard time-temperature shifting rules for this liquid. Details of the calculation of a traction curve for Hertz pressure of p_H=1.29 GPa and rolling velocity of U=2m/s and film thickness of h=0.177 μm are below.

We represent the variation of low shear viscosity with pressure by the Dolittle[3] equation,

$$\mu(\mathrm{p}) = \mu_o \exp\left[B \frac{v_{occ}}{v_o} \left(\frac{1}{\frac{v}{v_o} - \frac{v_{occ}}{v_o}} - \frac{1}{1 - \frac{v_{occ}}{v_o}} \right) \right] \quad (1)$$

where v is volume, v_o is volume at p=0, and v_{occ} is the occupied volume, independent of pressure. The variation of volume with pressure has been extrapolated to high-pressure from measurements to 0.35 GPa using the Tait[3] equation.

$$v/v_o = 1 - \frac{1}{K_o^{'}+1} \ln\left[1 + \frac{p}{K_o}\left(1 + K_o^{'}\right) \right] \quad (2)$$

A least squares regression of volume and viscosity data together resulted in K_o =0.907 GPa, $K_o^{'} = 13.7$, $v_{occ}/v_o = 0.669$, $B = 4.10$, and $\mu_o = 12.9\,\mathrm{m\,Pas}$.

We represent constitutive behavior by the shifted Carreau equation for viscosity

$$\eta(\dot{\gamma},\mathrm{p})=\mu\left[1+\left(\dot{\gamma}\lambda_{\mathrm{R}}\frac{\mu}{\mu_{\mathrm{R}}}\frac{\mathrm{T_R}}{\mathrm{T}}\frac{\mathrm{v}}{\mathrm{v_R}}\right)^2\right]^{(\mathrm{n}-1)/2} \tag{3}$$

where μ_R and λ_R are the viscosity and the relaxation time at T_R=311°K(38°C) and ambient pressure and $\dot{\gamma}$ is shear rate. From published[2] NEMD and experimental measurements $\mu_R = 15.6\,\mathrm{mPa\cdot s}$, $\lambda_R = 2.26\times10^{-9}\,\mathrm{s}$, and n=0.463. For v/v_R we substitute v/v_o from equation (2) and μ is calculated from equation (1).

The Newtonian limit in terms of shear stress is, from equation (3), always greater than 1.5 MPa. Therefore, a Newtonian film thickness calculation is appropriate and the Dowson-Hamrock[4] formula for central film thickness was used to arrive at h=0.177 μm. The shear rate can be calculated from

$$\dot{\gamma}=\frac{\mathrm{U}\Sigma}{\mathrm{h}} \tag{4}$$

where Σ is the contact slide to roll ratio, assuming a uniform value of h over the Hertz contact area.

The average contact shear stress results from integration of the local stress, τ, over the contact area,

$$\bar{\tau}=\int_o^1 2\mathrm{r}\tau\mathrm{dr} \tag{5}$$

for dimensionless contact radius, o < r < 1. For point contact the average pressure is $\bar{\mathrm{p}} = 2/3\,\mathrm{p_H}$ and the traction coefficient is simply $\bar{\tau}/\bar{\mathrm{p}}$. We assume that the pressure distribution is identical to that of the unlubricated Hertz contact.

$$\mathrm{p}=\mathrm{p_H}\left(1-\mathrm{r}^2\right)^{\frac{1}{2}} \tag{6}$$

First, we calculate traction for the Newtonian and Carreau cases where

$$\tau=\mu(\mathrm{p})\dot{\gamma} \tag{7}$$

and

$$\tau=\eta(\mathrm{p},\,\dot{\gamma})\dot{\gamma} \tag{8}$$

respectively. The traction curves for these cases are indicated in the figure.

We know from experimental measurement that at sufficiently large shear stress, τ, relative to the pressure, p, the deformation will localize limiting the magnitude of the shear stress. This has been shown in both experimental flow visualization[5] and molecular simulation[6]. The ratio of $\tau/\mathrm{p}=\Lambda$ that limits the shear stress was found from a traction measurement at p_H=1.93 GPa where the traction coefficient reached a plateau at 0.075. Two additional curves are plotted in the figure for Newtonian response with limiting shear stress

$$\tau=\min\left[\mu\dot{\gamma},\Lambda\mathrm{p}\right] \tag{9}$$

and Carreau with limiting stress

$$\tau=\min\left[\eta\dot{\gamma},\Lambda\mathrm{p}\right] \tag{10}$$

with Λ=0.075.

As shown in the figure, Carreau behavior captures the low sliding speed traction very well and with a limit to the shear stress it describes all of the measured traction.

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