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Pressure dependence of zero-shear viscosity by MD simulations

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Green-Kubo zero-shear viscosity calculations were carried out by performing classical MD simulations and computing time integrals over block averages of correlation functions for various pressure tensor elements. It was found that the Green-Kubo viscosity formula applied to molecular systems at various pressures provides valuable data for the investigation of the rheological properties of alkanes.

Keywords: lubricant/surface interaction, rheology of lubricants, molecular lubrication

1. Introduction

The Green-Kubo method [1] for calculating viscosities at zero-shear rate of liquid alkanes by means of molecular dynamics (MD) has been applied. Within this work, the common study of simulating viscosities close to ambient pressure has been extended to pressures relevant for studies of elastohydrodynamic lubrication (EHL) from 0.1 to 1000 MPa.

2. Computational details

The equilibration of investigated tribo-rheological systems has been traced by using the Hellinger metric for the time-dependent density distribution function for the one third of the sum of the off-diagonal pressure tensor components. In order to elucidate the influence of the chemical structure, rotational relaxation times were calculated by autocorrelating normalized intramolecular positions and fitting them to an exponentially decaying model. In addition, the partial contributions to the overall pressure tensor used for calculating the viscosity were examined separately to provide additional information about the structural influence.

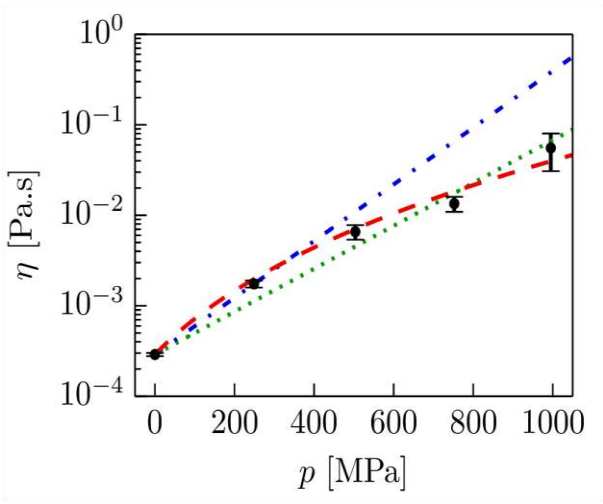

Figure 1: Pressure dependence of zero-shear viscosity for n-octane from MD simulations. Dotted (green) and dot-dashed (blue) lines stand for Barus' fittings, and the dashed (red) line for the Roelands' fitting, respectively.

3. Results and discussion

It was found that MD results obtained for normal alkanes are in good agreement with experimental measurements, while viscosities of branched alkanes are systematically overestimated. Furthermore, the pressure dependence of the calculated zero-shear viscosities is well described by Roelands' pressure viscosity relation [2]. Analysis of different contributions to the pressure tensor showed that in contrast to the normal alkanes, the pressure tensor contribution due to bonds dominates over the angle contributions in branched alkanes.

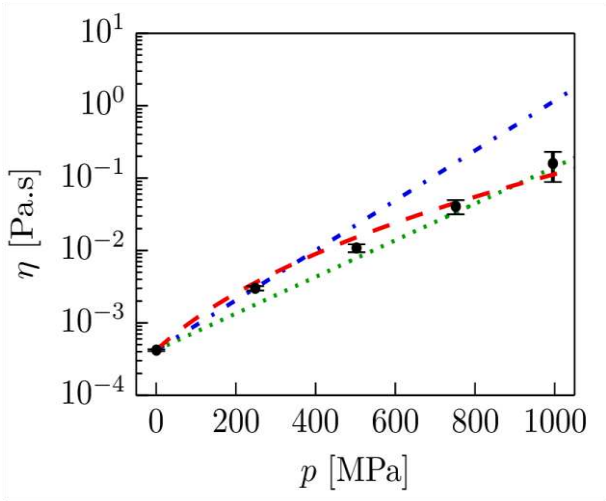

Figure 2: As in Fig. 1 for i-octane.

4. Acknowledgments

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5. References

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