Lubrication aspects of Cycloaliphatic rings

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Abstract: Esters of long-chain unsaturated fatty acids with a variety of alcohols, both linear and branched, are extensively used in the lubricant industry today. The work presents a combined experimental and molecular dynamic simulation (MDS) study to explore the influence of cycloaliphatic moieties on the lubrication behaviour of such long-chain unsaturated fatty acid esters. The study extends the generally accepted principle that disruptions to linearity may favourably enhance tribological properties. These disruptive structural features have been introduced by synthesizing the most strained three-membered heterocyclic rings (epoxy and thiirane) containing oxygen, sulfur, and least strained cyclohexyl moieties in the backbone of oleic acid esters. The synthesized lubricants were then subjected to physicochemical characterization. The structure-property relationships are developed by investigating their tribological characteristics.

Introduction: Earlier findings on lubricated contacts suggest that apart from physical properties (density, viscosity, and volatility), the molecular properties (i.e., molecular shape, size, polarity, and lubricating film thickness) and the surface characteristics are very crucial in predicting the performance of lubricated contacts. The interfacial properties arising from substrates and the molecular structure of lubricants are less ventured in machine Tribology. Therefore, this work is intended to study the impact of molecular structural variations (developed by generating homocyclic and heterocyclic moieties at the molecular backbone of long-chain esters) on friction and wear in an elliptical contact (ball-on-roller geometry). Further, these developed esters are applied at the interface of commonly used engineering substrates (Stainless steel, Aluminium, Phosphor Bronze, and Brass) and their tribo-performance explored in circular contact (ball-on-disc geometry). The evolution of molecular characteristics (binding energy, adsorption energy, diffusion coefficient, confined shear, and radial distribution function) with time is further related to the experimental results.

Results: Lubricants containing heterocyclic moieties show enhanced antifriction and anti-wear characteristicswhen compared with their homocyclic counterparts. This can be attributed to the molecular time evolution of the system which displays strong affinity of esters containing heterocyclic moieties in its backbone towards the iron substrate.

The wetting ability of heterocyclic moieties over common engineering substrates is much better than homocyclic ones. The improved performance can be attributed to the close packing and stearic factors that allow heterocyclic moieties to spread better than homocyclic ones.

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