The Molecular Modeling and Design of High Performance Biodegradable Lubricants

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The limited availability and rising cost of petroleum-based products has generated considerable interest in finding alternative, renewable sources. Industrial lubricants derived from vegetable oils provide a promising alternative to petroleum-based products. Unlike petroleum oils they are a naturally occurring, renewable, and biodegradable resource. Vegetable oils in the natural form, however, have had limited use as industrial fluids because of their oxidative stability, low temperature properties, and degradation under severe conditions of temperature, pressure, and shear stress.

In order to formulate vegetable oils with optimal lubrication characteristics, the influence of the individual molecular components on the overall oil properties must be understood. Vegetable oils are essentially mixtures of triacylglycerols. Although triacylglycerols are naturally abundant, the effect of molecular structure on their physical properties is not well understood. Computer simulations are used to directly relate molecular architecture to physical properties and improve our knowledge of this important class of materials.

We present our findings on the computational prediction of the transport coefficients, including viscosity and gel formation, of triacylglycerols and vegetable oil mixtures using both coarse grained and united atom force field representations. A systematic approach used for creating these force fields is presented. As shown in Figure 1 the results of atomistic and coarse grained simulations are in good agreement with experiment. In particular, the gel transitions predicted by our simulations are shown to be in remarkable agreement with experimental pour point data. The effect of molecular architecture on physical properties has been investigated for triacylglycerols that are either difficult to isolate in vegetable oils or are chemically modified, thereby providing principles for the rational design of new lubricants.

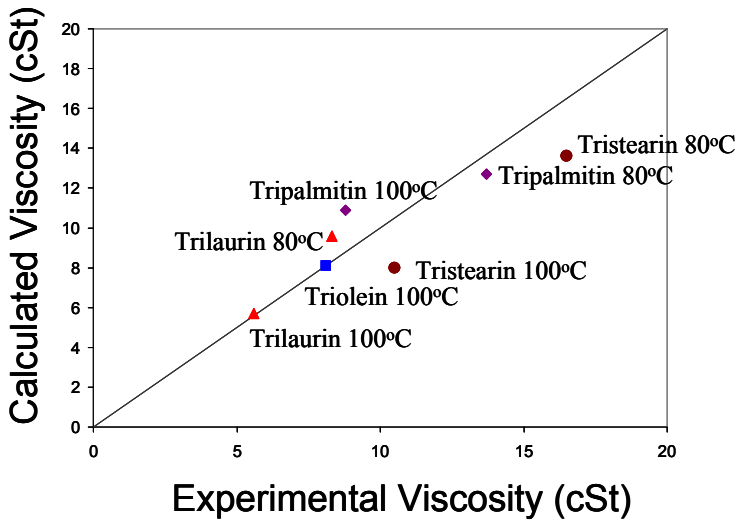

Figure 1: Comparison of experimental and calculated viscosities of several different triacylglycerols. (Results from A. K. Sum *et al.* J. Phys. Chem. B 107 (51) 14443-14451.)