

Effect of molecular architecture on the effectiveness of a Viscosity Index Improver under shear

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Viscosity modifiers (VMs) additives, which are commonly polymeric in nature, are added to lubricants to reduce its viscosity dependence on temperature. This allows a single lubricant formulation to be used in a wide range of conditions. The behaviour of these polymeric additives depends on the shear rate and temperature that they are subjected to. In this study, dissipative particle dynamics (DPD), a coarse-grained mesoscopic simulation technique, is used to investigate the effect of VM architecture on the rheology and viscosity-temperature dependence of the lubricant under elastohydrodynamic conditions. The effect of changing architecture and chemical composition on the size of the polymer with increasing solubility will be quantified, and how this dictates the effectiveness of the VM under shear is investigated.

Keywords: viscosity modifiers, polymer architecture, dissipative particle dynamics, elastohydrodynamic lubrication.

1. Introduction

Viscosity modifiers (VMs) additives are used to reduce the lubricant's sensitivity to temperature, which is crucial to the promotion of the reliability, efficiency and durability of the engineering components. A thorough understanding of how the VMs affect the rheology and viscosity of the lubricant will allow us to design more effective VMs [1]. This work aims to understand how polymer architecture and composition affects the effectiveness of a VM additive. This will be done by assessing the size of the polymer by means of the radius of gyration, R_g , hydrodynamic radius, R_h , and measuring the shear viscosity of the system.

2. Methods

In order to model the effect of changing architecture on the polymer's behaviour, the coarse-grained mesoscopic simulation technique, dissipative particle dynamics (DPD) was used [2]. DPD simulations allow for the longer timescale analysis of the mesoscopic system.

2.1. Simulation software.

Simulations were run using the open source software LAMMPS [3] and the system images were visualized with OVITO [4].

2.2. Simulation set up details.

Simulations are under an NVT ensemble (constant number of molecules, volume and temperature). A box size of 100x100x100 unit length is used, where all units are in reduced units. The mass of the DPD beads $m = 1$ and the density of the system, $\rho = 3$. All the polymer chains are length $N = 301$ DPD beads, with a total of 190 polymer chains. The interaction parameters are varied depending on the polymer system. The non-dimensional temperature, $k_b T = 1$, was used

2.3. Boundary conditions.

In equilibrium conditions, periodic boundary conditions are used.

In shear conditions, we use Lees-Edwards boundary conditions [5]. Here, a shear rate is imposed by inducing a velocity gradient through the modification of the periodic boundary conditions.

3. Discussion

Using DPD, the shear flow of the lubricant with varying polymer additives was investigated. Using different architectures, such as linear and star polymers, the effect of coil size on the viscosity enhancement power of the polymer, and how architecture changes this was studied. Moreover, a range of shear rates were investigated to understand shear thinning behaviour.

In addition, using varying configurations (e.g. block and alternating) of copolymers, i.e. $A_n B_m$ polymers, where A and B monomers have varying polymer-solvent interactions, the effect of aggregation on shear flow and the effectiveness of the VM was investigated.

4. References

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