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Numerical study of lubrication with nematic liquid crystals

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ABSTRACT

Liquid Crystals (LCs) are anisotropic viscoelastic materials; the combination of fluid-like flow with crystal-like anisotropy makes its phases interesting as modifiers of interfacial behavior when applied as lubricants. The ability of liquid crystalline materials to form ordered boundary layers with good load-carrying capacity, and to lower the friction coefficients, wear rates and contact temperatures of sliding surfaces, thus contributing to increase the components service life and save energy has been widely demonstrated. Friction is reduced by three to five times when nematic LCs are used over conventional oil.

The objective of this research is to study the lubrication with nematic LCs using modeling and numerical simulations. LCs are hierarchically structured materials so the computational design involves challenges, like the disparity between the length and time scales. The Reynolds scaling analysis was applied to the tensorial the Landau-de Gennes (LdG) theory to derive the simplified equations of lubrication theory. The full set of equations from the LdG theory for the liquid crystalline microstructure along with continuity and momentum equations with a modified stress tensor which accounts for the viscoelastic contribution, were solved simultaneously using General PDE (Partial Differential Equations) and Laminar Flow modules of COMSOL Multiphysics. The obtained simplified set of equations were validated by comparison with the solution obtained from the complete set of equations.

The parametric studies were conducted to understand the effect of different parameters on lubrication performance and on the orientation profiles. These studies involved changes in the balance of short-range elasticity, long range elasticity, and viscous forces and their effect on the orientation tensor and therefore the orientation. The effect of the coupling between the structure and the flow on the lubrication performance was also investigated.