Shear thinning in glycerol as a green lubricant: Atomic-scale overview by molecular dynamics simulation

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Given that friction accounts for about a quarter of energy losses in industrial systems, it is essential to seek satisfactory lubrication solutions. This issue becomes even more prominent when we know that applying oil-based lubricants is generally associated with considerable environmental risks. Glycerol-based lubricants are proper alternatives to oil-based and conventional green lubricants. In this study, the pressure-viscosity coefficient of pure glycerol is achieved separately by equilibrium and non-equilibrium molecular dynamics (MD) simulation. It is demonstrated that the pressure-viscosity coefficient obtained by the non-equilibrium MD is in good agreement with the experimental results. Furthermore, by implementing non-equilibrium MD simulation, the viscosity of pure glycerol is calculated at different pressure values and strain rates. It is inferred that shear thinning occurs in pure glycerol by decreasing the strain rate. The proposed computational framework not only evaluates the alterations of the viscosity at a specified strain rate and pressure but also provides a basis for studying the behavior of aqueous solutions of glycerol at atomic scale.

Keywords: Green Lubricant, Glycerol Aqueous Solutions, Molecular Dynamics Simulation, Viscosity

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