STLE Tribology Frontiers Conference – Chicago 2019

Base Oil Friction Prediction under Severe Conditions from Molecular Dynamics Simulations

KEYWORDS

Lubrication, Friction, Molecular Dynamics

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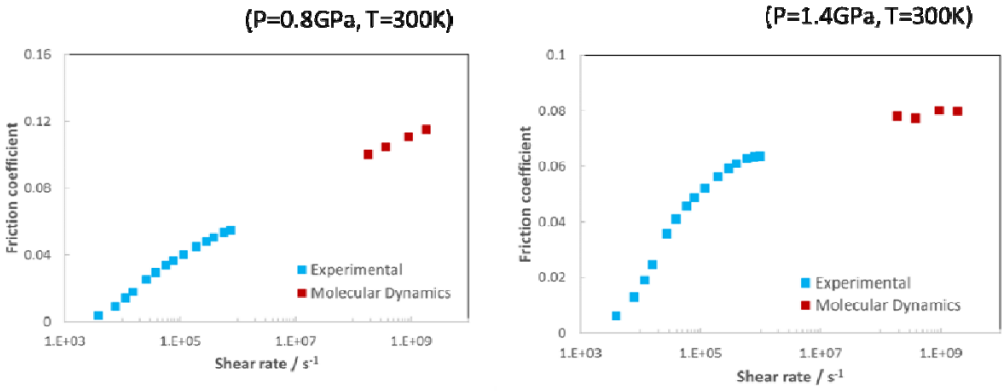
ABSTRACT

Film thickness prediction in elastohydrodynamic (EHD) lubrication regime benefits nowadays from efficient semi-analytical formula. This is still not the case for EHD friction because several physical behaviors interact simultaneously (fluid rheology, thermodynamics, shear heating, etc.). To identify the key mechanisms responsible for lubricated friction at the molecular scale, Molecular Dynamics simulations are proposed. The material studied is a commercial base oil of which the chemical composition is determined. At equilibrium (without shear), the thermodynamic state of the lubricant is identified. Under pressure, temperature and shear, friction evolves in different ways according to the thermodynamics state of the lubricant, from shear rate-dependent to shear rate-independent friction.

The calculated friction is then confronted to experimental results obtained from a ball-on-disc apparatus. As shown by [1] and [2] on pure liquids, independently of surface effects, the numerical prediction, though at very high shear rate, proves to be a very good extrapolation of experimental results also for this commercial base oil.



ACKNOWLEDGMENTS

This work was supported by the INSA Lyon-SKF Research Chair “Lubricated Interfaces for the Future”.

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