UNDERSTANDING ACTION MECHANISMS OF AMINE-BASED FRICTION MODIFIERS THROUGH MOLECULAR SIMULATIONS

Rafael Pereira de Matos [a,b*], Toni Massoud [a], Clotilde Minfray [a], Franck Dahlem [a], Sophie Loehlé [b], Manami Sato [c], Nozomu Hatakeyama [c], Akira Miyamoto [c], Manuel Cobián [a]

* rafael.pereira-de-matos@doctorant.ec-lyon.fr

[a] Laboratoire de Tribologie et Dynamique des Systèmes, Ecole Centrale de Lyon, 36 avenue Guy de Collongue, 69134 Ecully Cedex, France

[b] TOTAL, Centre de Recherche de Solaize, BP22 – 69360, Solaize Cedex, France

[c] New Industry Creation Hatchery Center, Tohoku University, 6-6-10 Aoba, Aramaki, Aoba-ku, 980-8579, Sendai, Japan

KEYWORDS

Organic friction modifiers, amines, iron-based surfaces, Molecular Dynamics

ABSTRACT

Friction-modifier (FM) additives of thermal engine lubricants have been beneficial in reducing friction between contacting surfaces [1]. In particular, organic nitrogen-containing compounds such as fatty amines seem to be promising additives. Besides their tribological performance, they are compatible with exhaust aftertreatment systems due their sulfur- and phosphorus-free chemical composition.

In this computational study, we have investigated the mechanisms of action of amine-based FM using electronic structure and Molecular Dynamics calculations. An α-iron oxide Fe_2O_3 surface was used as rubbing substrate model. The aim was to better understand the impact of the chemical structure of these additives on the thermal film formation and eventually on their tribological behavior.

REFERENCES

[1] Tang, Z., Li, S. (2014), "A review of recent developments of friction modifiers for liquid lubricants (2007-present)", Current Opinion in Solid State and Materials Science, 18, p. 119-139.