MD SIMULATIONS OF FRICTION AND WEAR OF FUEL SURROGATES

J.A. Harrison[a*], J.D. Schall[b], S. Maskey[a], B.H. Morrow [a]
*corresponding author email: jah@usna.edu
[a] United States Naval Academy, Chemistry Department,
572 Holloway Road, Annapolis, MD, 21402, USA
[b] Oakland University, Mechanical Engineering Department
Rochester, MI, 48309, USA

KEYWORDS

Fluid lubrication; Nanotribology; Friction; Wear

Keywords list:

- Friction
- Rheology
- Rolling contact fatigue
- Coating
- Lubricant additives
- Biotribology
- Mixed Lubrication
- Surface topography
- Experiments in tribology
- Physics of friction
- Texturation
- Wear
- Fretting
- Solid lubrication
- Fluid lubrication
- Tribofilms and 3rd bodies
- Hydrodynamic Lubrication
- EHL
- NanoTribology
- Modelling in tribology
- Contact and adhesion
- Everyday life tribology

ABSTRACT

The application of carbon-based coatings to engine components has become increasingly more common. Coatings, such as ultrananocrystalline diamond (UNCD) and amorphous carbon (a-C:H) can have a wide-range of properties but are generally attractive due to their wear resistance. At the same time, alternative fuels, such as Catalytic Hydrothermal Conversion Jet (CHCJ), diesel (CHCD) and others are being developed. Because these fuels are complex, surrogates for these fuels have been developed so that impacts of changes in composition on properties and combustion can be studied. To date, little effort has been devoted to the study of the interactions of these fuels with engine coatings. The results of molecular dynamics (MD) simulations using both the REBO+S and the ReaxFF potentials, that examine the interaction of two- and three-component CHCJ surrogates with carbon-based engine will be presented.

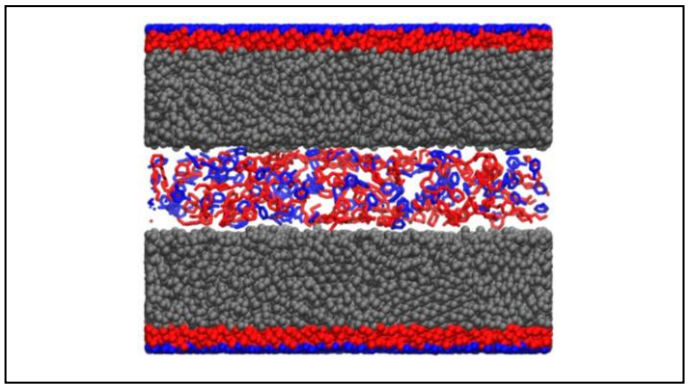

Fig.1 This is a snapshot of a molecular dynamics simulation system. In this system, a 50:50 mixture of toluene (blue molecules) and butylcyclohexane (red molecules) are confined between two ultrananocrystalline, UNCD, coatings (gray spheres). Hydrogen atoms on the confined fuel molecules are not shown for clarity. The outer red and blue UNCD layers are thermostated and held rigid, respectively. The distance between the rigid layers is changed to control the load and the upper surface is slid to the right to simulate sliding.

Your abstract should be submitted **via the website**, http://leeds-lyon2019.sciencesconf.org/

ACKNOWLEDGMENTS

This work was partially supported by the Research Office at the United States Naval Academy and the Office of Naval Research.