June 2015 Highlights

ORNL Fuels, Engines, and Emissions Research Center

TECHNICAL HIGHLIGHTS

The Oak Ridge National Laboratory (ORNL) Partners on Advanced Research Projects Agency-Energy (ARPA-E) Project to Achieve 40% Efficiency in a Small Natural Gas Engine
ORNL is a partner with Michigan-based MAHLE Powertrain on a successful proposal that will be awarded $2.5 million in ARPA-E funding over 3 years. The team led by MAHLE Powertrain will design and develop a prototype 1kW internal combustion engine for third party evaluation at the end of the second project year. The proposed concept combines downsizing, novel fuel injection, lean combustion, and reduced friction to meet the efficiency target. Researchers in ORNL's Fuels, Engines & Emission Research Center (FEERC) will develop a novel low-temperature after-treatment system to reduce exhaust emissions. The ORNL proposal team included Mike Kass, Derek Splitter, Brian Kaul, Jim Szybist, Josh Pihl, and Dean Edwards.

ORNL's New Publication Provides New Insights into Role of Lubricant Anti-wear Additives on Form Tribofilms on Non-metallic Surfaces
Lubricant anti-wear additives are known to chemically interact with metallic surfaces to form a self- healing, wear-protection tribofilm. Their interactions with non-metallic surfaces are however less understood. Here we report recent findings on whether and how a zinc dialkyldithiophosphate (ZDDP) and a phosphonium–organophosphate ionic liquid (IL) form tribofilms on three hard coatings, AlMgB14– TiB2, TiB2, and diamond like carbon (a-C:H DLC), when sliding against a steel ball. Systematic characterization was conducted on the coating wear scars including top surface morphology imaging and elemental mapping, layer-by-layer chemical analysis, and cross section nanostructural examination. The ZDDP and IL tribofilms on the boride coatings are up to 50–70 nm thick with 75–80% surface coverage while the tribofilms on DLC were 25 nm thick and only covered 20–30% of the contact area. The presence of iron compounds in the tribofilms suggests a critical role for wear debris in tribofilm formation. Oxidation products of TiB2 were detected in the tribofilms, while no involvement of the DLC surface in tribofilm formation was observed. Results suggest that wear debris digestion and contact surface reaction both are critical in tribofilm formation: the former process is responsible in forming the bulk of the tribofilm and the latter provides strong bonding of the tribofilm to the contact surface.
Reference: J. Qu, H. M. Meyer III, Z.-B. Cai, C. Ma, and H. Luo, "Characterization of ZDDP and Ionic Liquid Tribofilms on Boride and DLC Coatings," pp. 1273–1285 in *Wear*, **332–333**, 2015.

Recent Study Discusses Complex Impact of Oil Temperature Change on Wear Rate Due to Associated Change in Oil Viscosity, Water Content, and Surface Oxidation
Tribological tests were conducted on an AISI A2 steel plate against an AISI 51200 steel ball lubricated by Society of Automotive Engineers (SAE) 0W30 and PAO 4 cSt base oils containing no additive package. Friction and wear behaviors were evaluated at room temperature (room temperature (RT), 23°C) and a series of elevated temperatures (75, 100, 125, and 175°C). The steady-state friction coefficient appeared to be proportional to the oil temperature, probably because reduced oil viscosity at a higher temperature caused more surface asperity collisions. In contrast, wear results did not follow the trend: the wear rate surprisingly decreased when the oil temperature increased from RT to 75–

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100°C, and then turned around to increase along with the temperature at above 100°C. Evidentially, there are other significant factors than just the oil viscosity that influence the wear process upon the temperature change. Wear scar morphology examination and surface chemical analysis revealed an oxide-containing surface film on the wear scars and higher oxide content and larger film coverage seemed to reduce the wear rate. Therefore, the wear mechanism is proposed as a combined effect of mechanical material removal and protective surface film formation: the former largely depending on oil viscosity that is inversely proportional to the temperature and the latter involving surface and wear debris oxidation that is promoted by temperature elevation as well as the water content (up to 100°C) in the oil.
Reference: Z.-B. Cai, Y. Zhou, and J. Qu, "Effect of Oil Temperature on Tribological Behavior of a Lubricated Steel-Steel Contact," pp. 1158–1163 in *Wear,* **332–333,** 2015.

FEERC Participates in Steering Committee for the United States (US)-China Clean Energy Research Centers (CERC)
FEERC Director Robert Wagner attended the invitation-only steering committee meeting for the US-CERC. Robert coordinates ORNL participation in the CERC on Clean Vehicles. The meeting was led by the Department of Energy (DOE) Secretary Moniz and China Minister of Science & Technology Wan with additional participants from the US and China governments, national laboratories, universities, and industry. The meeting closed with a signing ceremony which added a fourth CERC on energy and water.

High-Level or Noteworthy Visits

Invited Talks and Presentations

ORNL-General Motors (GM) Collaborative Efforts Presented at Oak Ridge Leadership Computing Facility (OLCF) Users' Meeting
Dean Edwards and Charles Finney of ORNL and Ron Grover and Tang-Wei Kuo of GM attended the OLCF Users' Meeting on June 22–25, 2015. While there, Ron Grover presented a poster entitled "Multi-Hole Injector Optimization for Spark-Ignited, Direct-Injection Gasoline Engines," which highlighted ORNL and GM's collaborative efforts utilizing DOE ASCR high-performance computing (HPC) resources at the OLCF (including Titan) to improve predictive modeling of gasoline direct-injection (GDI) sprays and accelerate the injector design process.

ORNL Invited to Environmental and Energy Study Institute (EESI) High Octane Fuels Briefing
Brian West of FEERC was invited to present recent results and outline ongoing high octane fuels research underway for the Bioenergy Technologies Office and Vehicle Technologies Office at a recent briefing in Washington. EESI sponsored the briefing to help educate attendees on the fuel economy, greenhouse gas, and petroleum displacement advantages of high-octane mid-level ethanol blends. Other speakers included the Honorable Tammy Duckworth (D-IL), Robert McCormick and Caley Johnson of the National Renewal Energy Laboratory (NREL), and Michael Wang of Argonne National Laboratory (ANL). The briefing was attended by 60 people including Congressional Staffers and was also simultaneously webcast. Oil Price Information Service (OPIS) and other media outlets have reported on the event.

FEERC Research Featured at 13th International Conference on Engines for Vehicles
FEERC research and insights on future fuels was featured at the invitation-only 13th International Conference on Engines for Vehicles held outside of Stoney Brook University in Long Island, New York. The event featured presentations and discussions from leaders in internal combustion research. The ORNL presentation put together by FEERC Director Robert Wagner, post-doc Adam Dempsey and researcher Scott Curran entitled "Directions in High Efficiency Engine Research and Future Fuel Opportunities" kicked off the technical sessions on the first day of the conference. Other presentations included leading researchers from industry, academia and the DOE national laboratories.

Strong FEERC Presence at 2015 DOE Vehicle Technologies Annual Merit Review
FEERC research was well represented at the recent DOE Annual Merit Review. This included thirteen oral presentations in the Advanced Combustion Engines R&D, Fuel and Lubricant Technologies R&D, and Technology Integration programs, an additional oral presentation in the Propulsions Materials program, and a poster presentation in the Vehicle and Systems

Simulation program, all presented by FEERC staff. FEERC staff also contributed to numerous additional research activities presented by our industry, university, and national lab partners.

Webinar on High Octane Fuels Features ORNL Researchers
Brian West and Tim Theiss along with NREL and ANL colleagues were invited to participate in a webinar sponsored by the 25x'25 Alliance. Brian and Tim presented recent results and outlined ongoing high octane fuels research underway for the Bioenergy Technologies Office and Vehicle Technologies Office. The 25x'25 Alliance is committed to biofuels advocacy, with a goal of replacing 25% of US energy use with renewables by 2025. The webinar highlighted the fuel economy, greenhouse gas, and petroleum displacement advantages of high-octane mid-level ethanol blends. Over 100 participants logged in for the webinar.

AWARDS

OUTREACH